Spectral Analysis of Stochastic Networks

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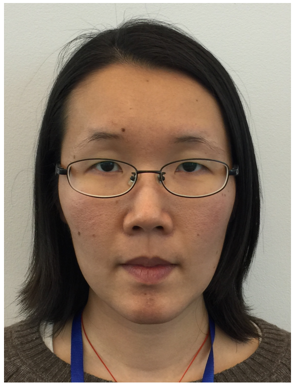
(joint work with Tingyue Gan (AMSC, UMD))



Workshop: Fluctuation—driven phenomena in non-equilibrium statistical mechanics,
Warwick University, UK, September 2015

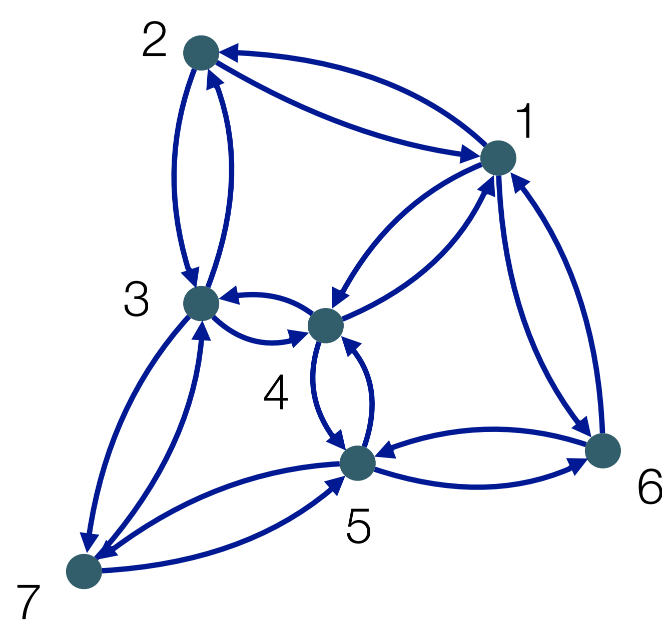
Networks with pairwise rates of the form $L_{ij} = a_{ij} \exp(-U_{ij} / T)$, T = a small parameter (temperature)

Time - reversible

1. Stochastic networks representing energy landscapes of atomic and molecular clusters and proteins (Wales's group (Cambridge Univ.))
2. Evolutionary genetics: fitness landscapes. (Kimura, Ewens, Gillespie) (A. Morozov & M. Manhart)
3. Markov State Model in Molecular Dynamics. (Schuette, Swope, Pande, Noe, etc)

Time - irreversible

1. Molecular motors. (Astumian (2005))
2. Aggregation of interacting particles.
3. Stochastically oscillating energy landscapes.

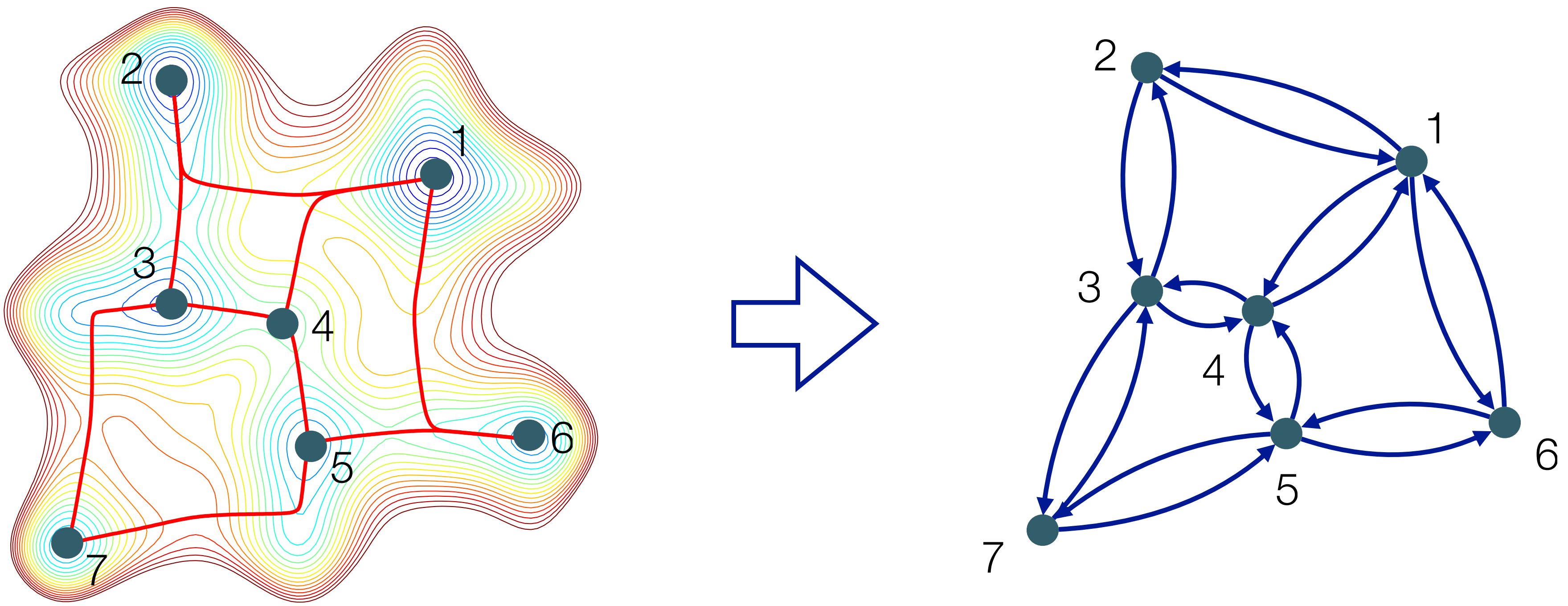


Reversible networks

$$U_{ij} = V_{ij} - V_i,$$

$$c_{ij} = \frac{c_{ij}}{c_i},$$

where $V_{ij} = V_{ji}, \quad k_{ij} = k_{ji}$



The generator matrix:

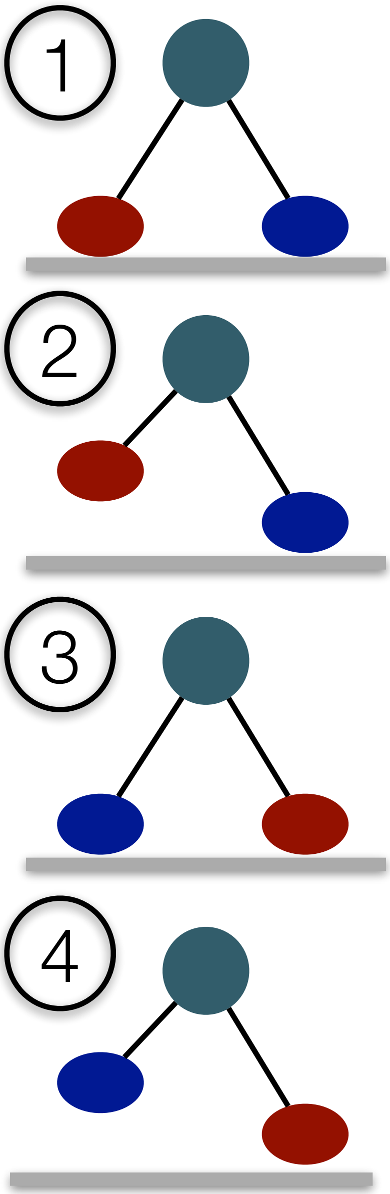
$$L_{ij} = \begin{cases} (k_{ij}/k_i) e^{-(V_{ij} - V_i)/T}, & i \sim j \\ 0, & \textit{otherwise} \end{cases}$$

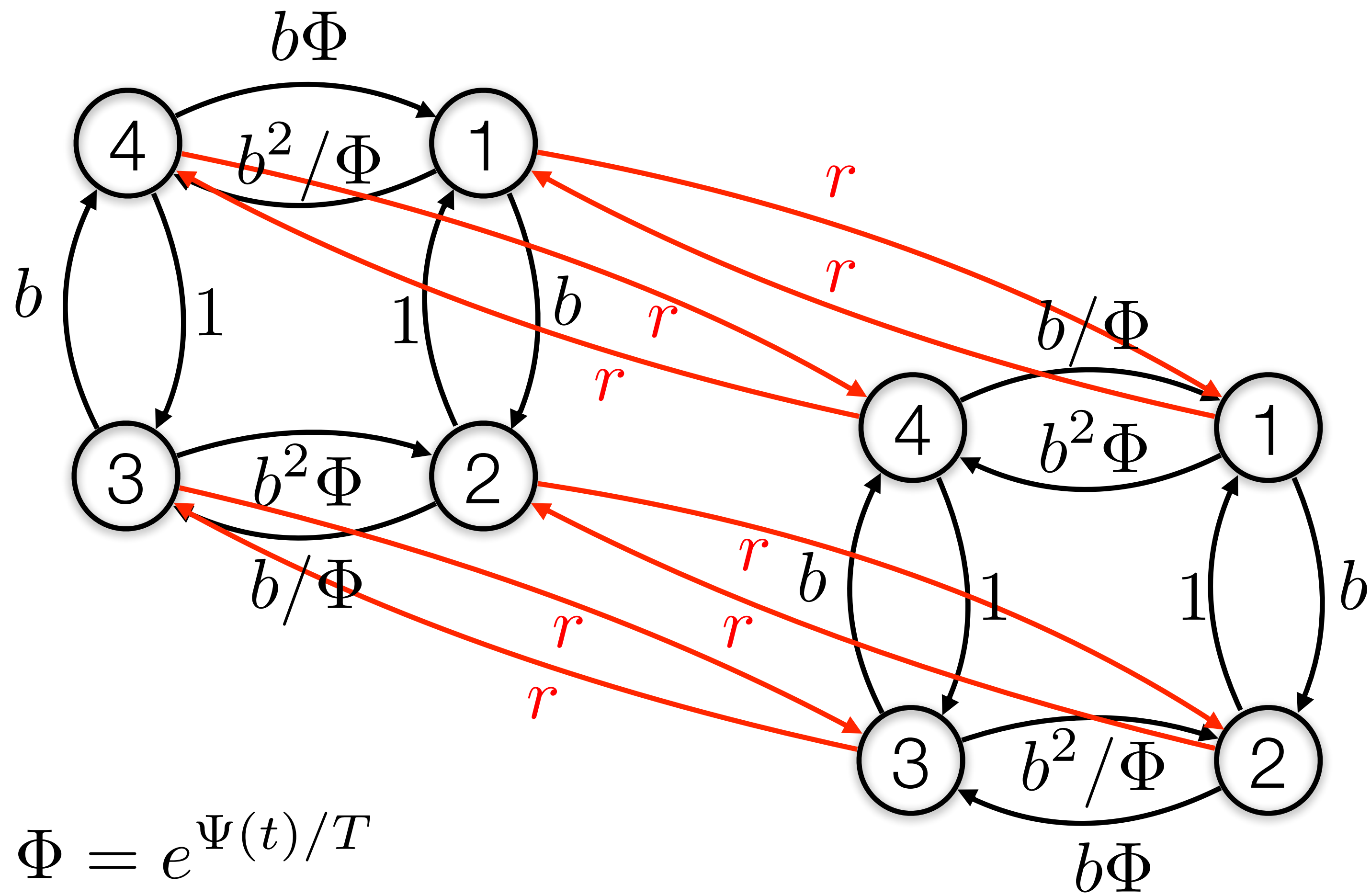
$$L_{ii} = -\sum_{j \neq i} L_{ij}$$

The invariant distribution:

$$\pi_i = k_i e^{-V_i/T}$$

Irreversible networks: Molecular motors
(Astumian, 2005)

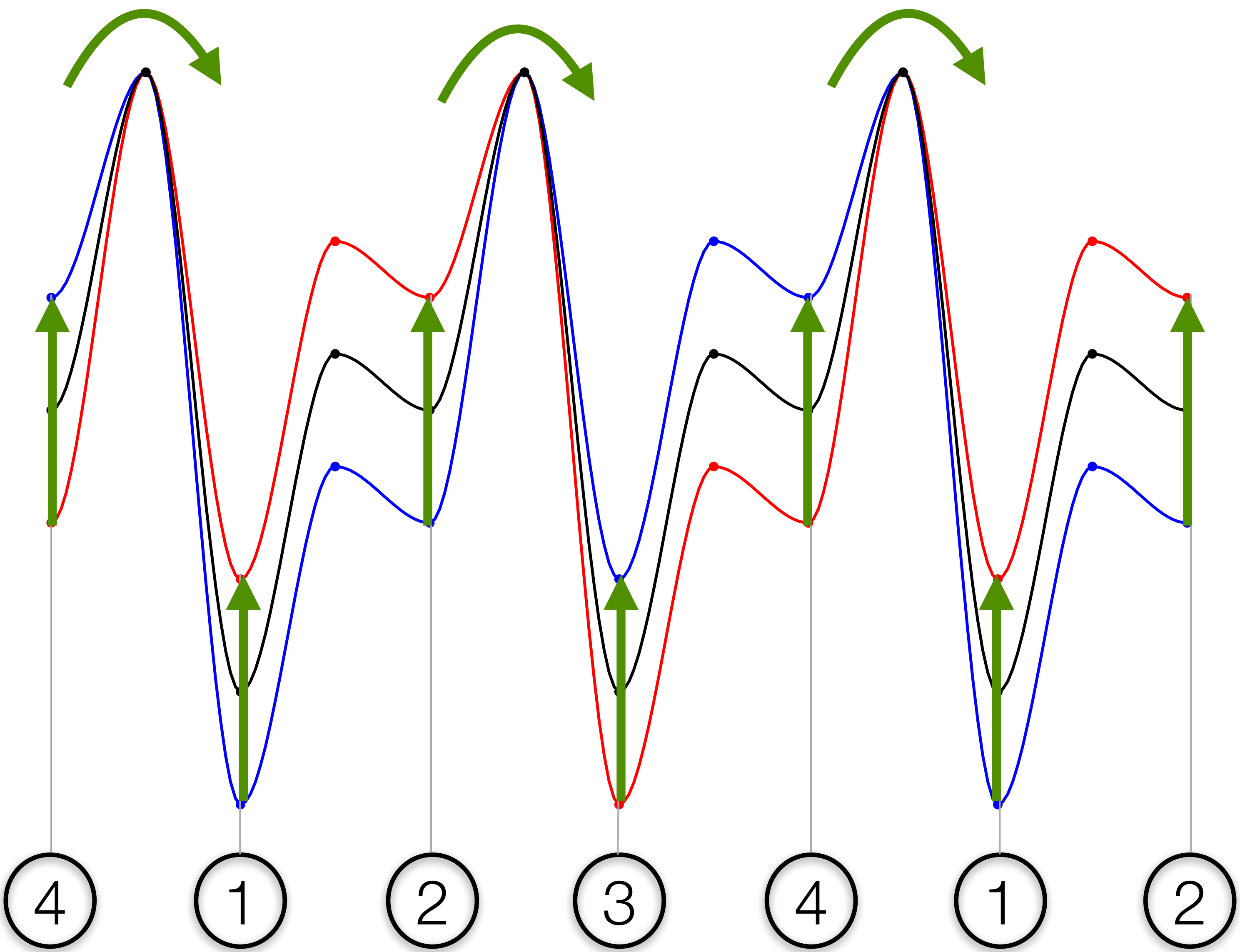




$\Phi = e^{\Psi(t)/T}$

Ψ switches between $+\Psi$ and $-\Psi$
with Poisson-distributed lifetime $r = Ae^{-a/T}$

Molecular motors, cont'd (Astumian, 2005)



black: $\Psi = 0$
blue: $\Psi > 0$
red: $\Psi < 0$

Significance of the spectral decomposition

$L = \Phi\Lambda\Psi \equiv \Phi\Lambda\Phi^{-1}$

- Understanding of the dynamics of the network: decompose it into a collection of processes with various time scales
- Extraction of quasi-invariant sets of states
- Building coarse-grained models

Interpretation of spectral decomposition

$$L = \Phi\Lambda\Psi \equiv \Phi\Lambda\Phi^{-1}$$

$$\Psi = \begin{bmatrix} \pi & \rightarrow \\ \psi_1 & \rightarrow \\ \cdots & \cdots \\ \psi_{n-1} & \rightarrow \end{bmatrix}$$

The matrix of left eigenvectors,

$$\pi = [\pi_1, \ldots, \pi_n]$$ = the invariant distribution

$$\Phi = \begin{bmatrix} e & \phi_1 & \ldots \phi_{n-1} \\ \downarrow & \downarrow & \ldots \downarrow \end{bmatrix}$$

The matrix of right eigenvectors,

$$e = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

$$\Lambda = \begin{bmatrix} 0 & & & \\ & z_1 & & \\ & & \ddots & \\ & & & z_{n-1} \end{bmatrix}$$

Eigenvalues: $z_k = -\lambda_k + i\mu_k$

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{n-1}$$

The Fokker-Planck equation or the Master equation

$$\frac{dp(t)}{dt} = p(t)L, \quad p(0) = p^0 = [p_1, \ldots, p_n]$$

The time evolution of the probability distribution

$$p(t) = p^0 e^{tL} = p^0 \Phi e^{t\Lambda} \Psi = \pi + \sum_{k=1}^{n-1} (p_0 \phi_k)\, e^{z_k t} \psi_k$$

Time evolution of the probability distribution

$$p(t) = \pi + \sum_{k=1}^{n-1} \boxed{(p_0 \phi_k)}\, e^{-\lambda_k t + i\mu_k t} \boxed{\psi_k}$$

Projection of
the initial distribution
onto right eigenvector

Left eigenvector

Left eigenvector ψ_k decays **uniformly** across the network with rate λ_k

For time-reversible networks:

$L = P^{-1}Q$, where $P = diag\{\pi_1, \ldots, \pi_n\}$, Q is symmetric

Right eigenvectors: $\Phi = [\phi_0, \ldots, \phi_{n-1}]$

Left eigenvectors: $P\Phi = [P\phi_0, \ldots, P\phi_{n-1}]$

Right eigenvector $\alpha_k \phi_k$ = proportion by which the states are over- or under-populated in the perturbed distribution $\pi + \alpha_k P \phi_k$

Difficulties in computing spectral decomposition

- The generator matrix is large: L in n-by-n, $n = 10^p$, $p = 4,5,6,\ldots$
- The pairwise rates U_{ij} can vary by tens of orders of magnitude
- No special structure
- Even if we succeed, the results would be hard to interpret

Idea

Step 1: compute the asymptotic spectral decomposition

Step 2: continue eigenpairs of interest to finite temperatures

The goal

- To develop an efficient algorithm for computing the zero-temperature asymptotics for eigenvalues and eigenvectors of the generator matrices
- To develop efficient continuation techniques
- Applications to large and complex networks representing energy landscapes

Asymptotics for eigenvalues and eigenvectors

Asymptotics for eigenvalues

A. Wentzell, 1972

For a continuous-time Markov chain
with pairwise rates of the form

$$L_{ij} \sim e^{-U_{ij}/T}$$

if all optimal W-graphs are unique,
eigenvalues of the generator matrix are

$$0 > -\lambda_1 \geq \ldots \geq -\lambda_{N-1}$$

$$\lambda_k \asymp \exp(-\Delta_k/T)$$

$$\Delta_k = V^{(k)} - V^{(k+1)}$$

$$V^{(k)} = \sum_{(i \to j) \in g_k^*} U_{ij}$$

where g_k^* is the optimal W-graph
with *k* sinks

T. Gan, C., 2015

For a continuous-time Markov chain
with pairwise rates of the form

$$L_{ij} = a_{ij} e^{-U_{ij}/T}$$

if all optimal W-graphs are unique,
eigenvalues of the generator matrix are

$$0 > -\lambda_1 \geq \ldots \geq -\lambda_{N-1}$$

$$\lambda_k = A_k \exp(-\Delta_k/T)$$

$$\Delta_k = V^{(k)} - V^{(k+1)}$$

$$V^{(k)} = \sum_{(i \to j) \in g_k^*} U_{ij}$$

$$A_k = \frac{\prod_{i \to j \in g_k^*} U_{ij}}{\prod_{i \to j \in g_{k+1}^*} U_{ij}} + o(1)$$

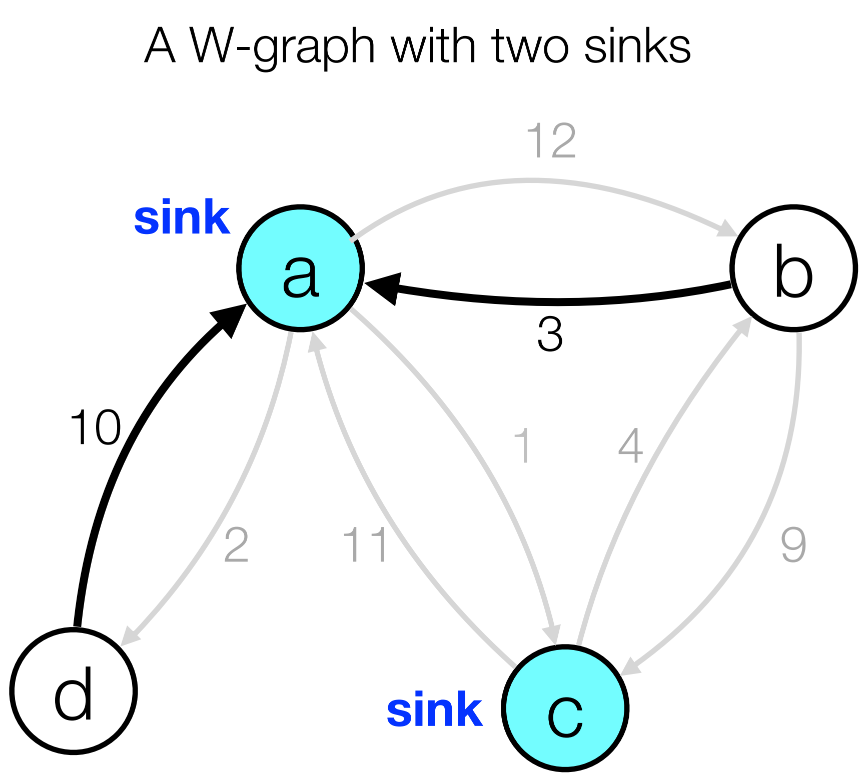
W-graphs (Wentzell, 1972)

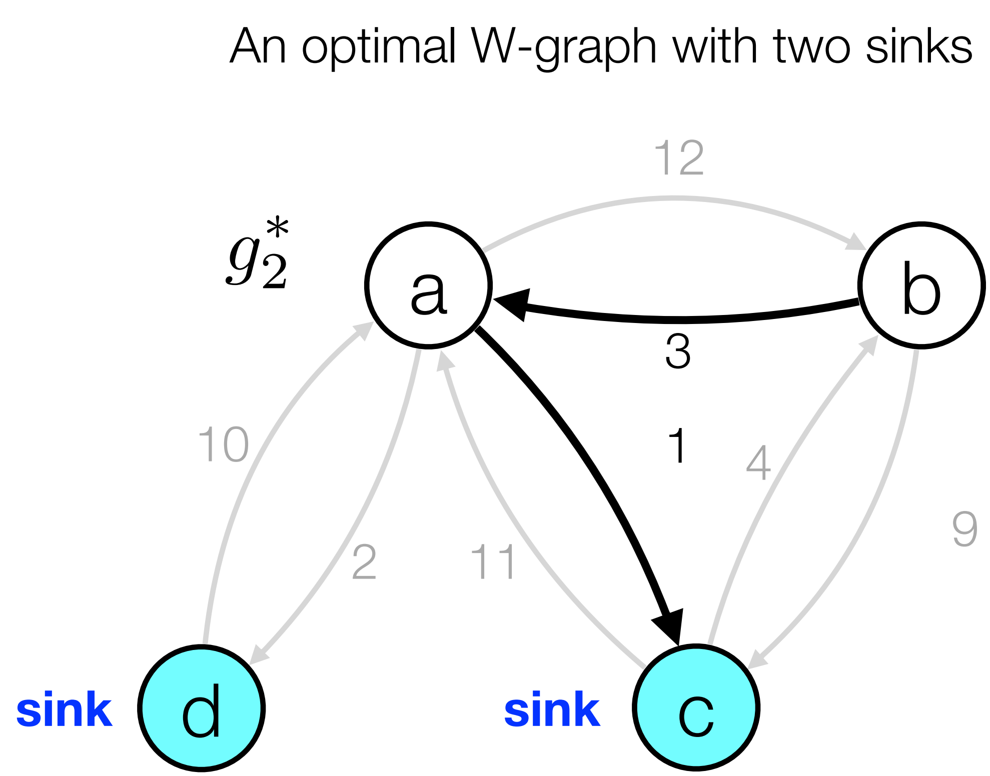
Definition. Let $G(S,A,U)$ be a weighted directed graph.
A W-graph with k sinks is its subgraph satisfying:

(1) any sink has no outgoing arcs; any non-sink has exactly one outgoing arc;

(2) the graph has no cycles.

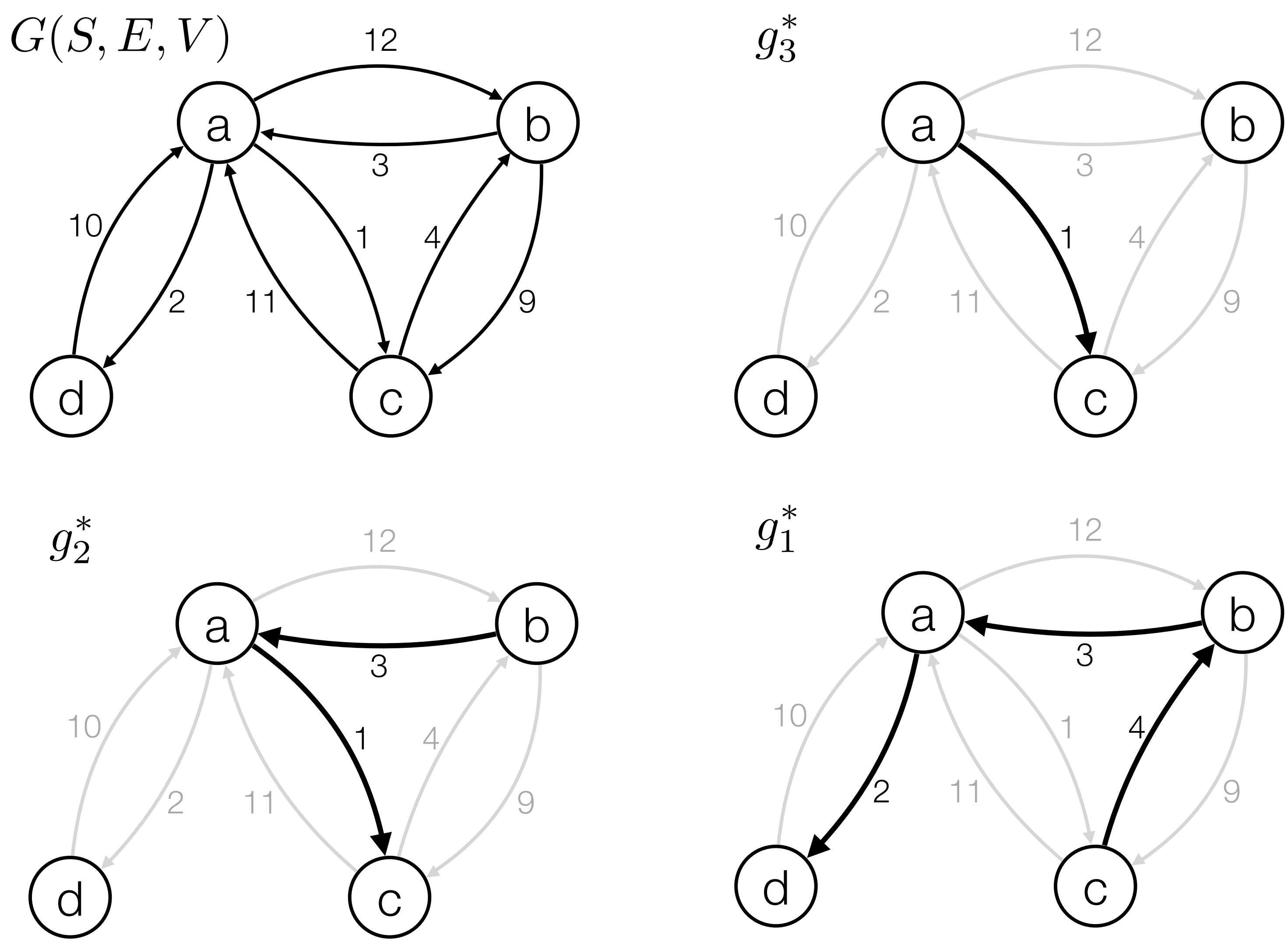
Example





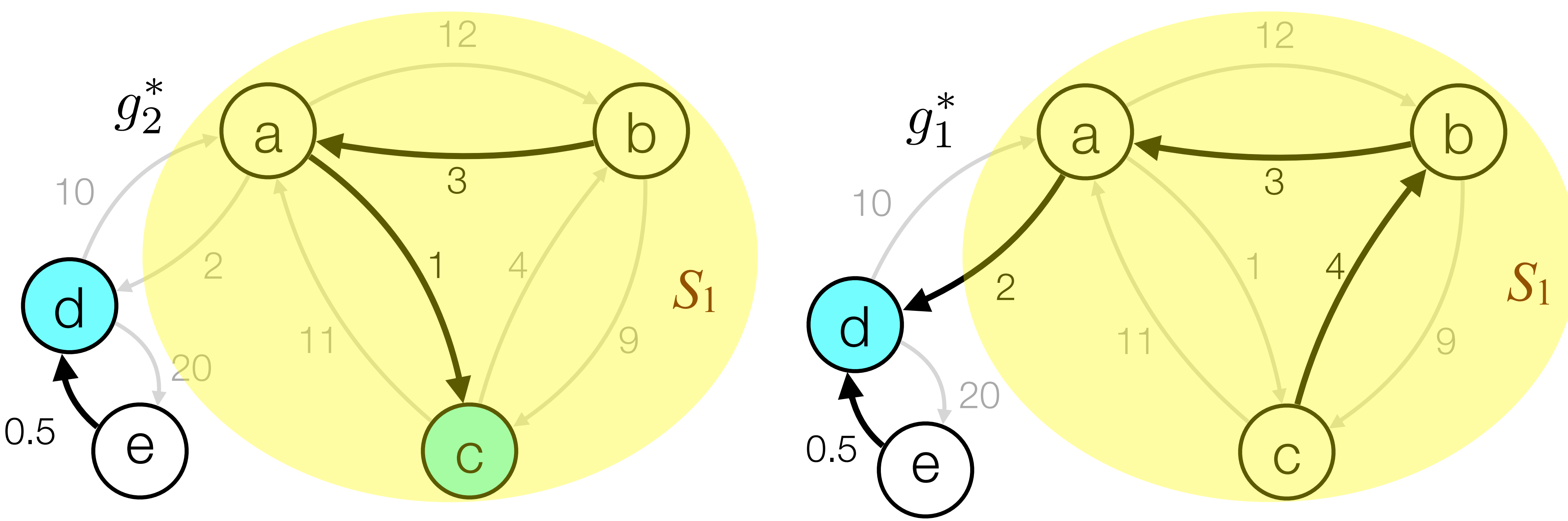
Optimal W-graphs with *k* sinks:

$\sum_{(i\to j)\in g} U_{ij}$ is minimized with respect to both *k* sinks and *n*-*k* arcs

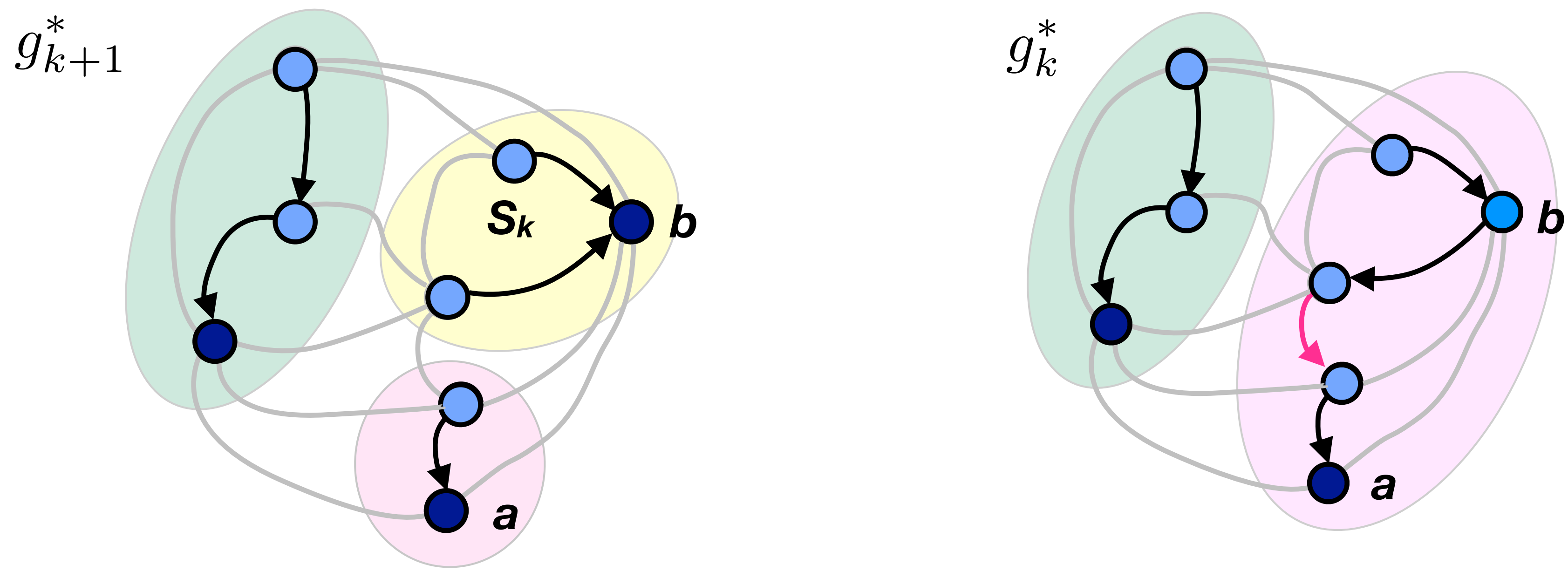


Nested property (Gan, C., 2015)

- {The set of sinks of g_k^* } $\subset$ {The set of sinks of g_{k+1}^* }
- There exists a connected component S_k of g_{k+1}^* whose set of vertices contains no sink of g_k^*.
- The sets of arcs connecting vertices $S \backslash S_k$ in g_k^* and g_{k+1}^* coincide.
- In g_k^*, there is a single arc from S_k to $S \backslash S_k$



Asymptotics for eigenvectors
(under assumption that ll optimal W-graphs are unique)



Right eigenvectors:

$$\phi^k_i = \begin{cases} 1, & i \in S_k \\ 0, & i \notin S_k \end{cases}$$

Time- reversible case:
Justification: Bovier, Eckort, Gayrard, Klein, early 2000's

Left eigenvectors:

$$\psi^k_i = \begin{cases} 1, & i = b \\ -1, & i = a, \\ 0, & i \notin \{a, b\} \end{cases}$$

Time - irreversible case:
Justification:
Cameron, Gan, 2015

Algorithms on graphs for finding asymptotic for eigenvectors and eigenvalues

Algorithms for computing asymptotic spectra

Algorithm 1
(Cameron, 2014)

Valid for time-reversible networks

Precompute the minimum spanning tree

Order of computation: from smallest to largest

(Cameron, NHM, 9, 3, 383-416 (2014), arXiv:1402.2869; Cameron. J. Chem. Phys., 141,

NEW! **Algorithm 2**
(Tingyue Gan, Cameron 2015)

Time-reversibility is not assumed

A **single-sweep** algorithm
(motivation: Chi-Liu/Edmond's algorithm for optimum branching for a directed graph with a selected root)

Order of computation: from largest to smallest

In preparation

The single-sweep algorithm (Cameron, Gan., 2015)

Input:

list of arcs with weights
and prefactors

$$1 \to i_1 : U_{1i_1}, \quad k_{1i_1}$$

$\vdots$

$$1 \to i_{n_1} : U_{1i_{n_1}}, \quad k_{1i_{n_1}}$$

$\vdots$

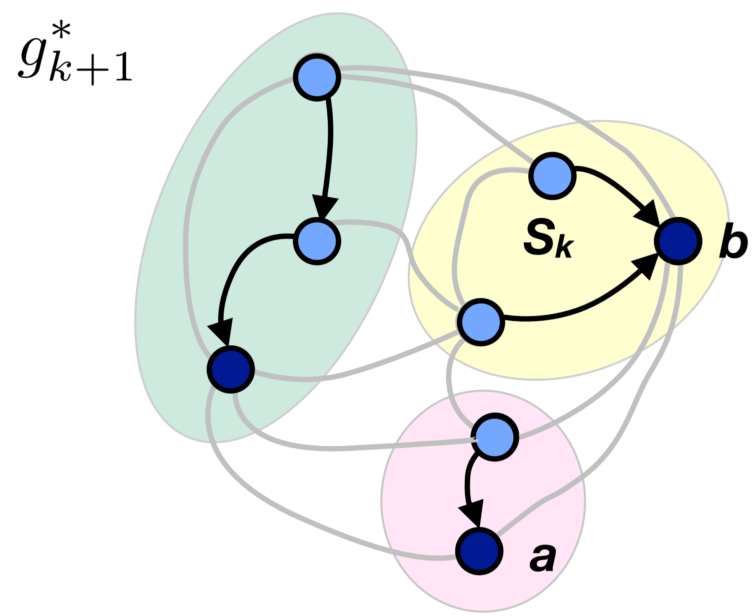
$$N \to p_1 : U_{1p_1}, \quad k_{1p_1}$$

$\vdots$

$$1 \to p_{n_N} : U_{1p_{n_N}}, \quad k_{1p_{n_N}}$$

Output:

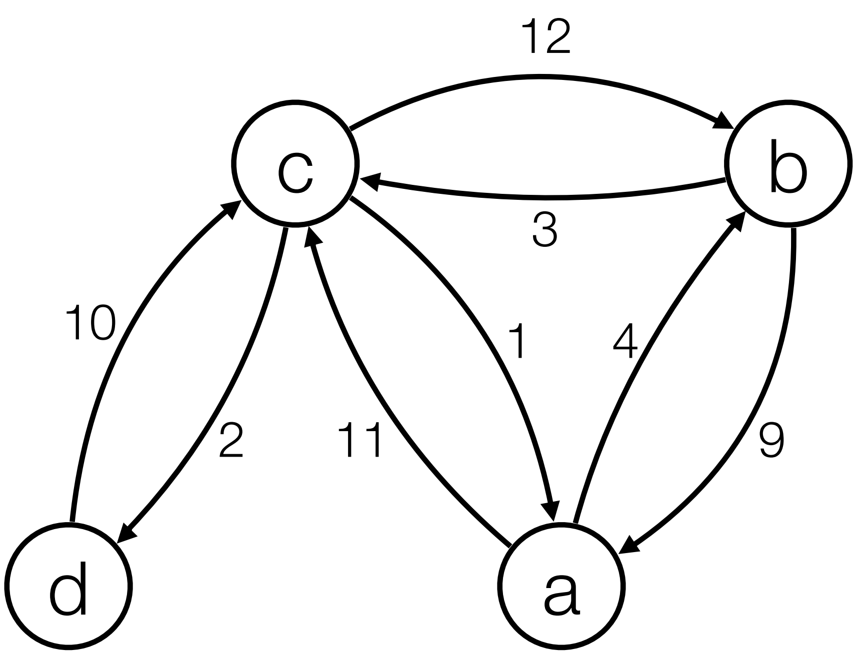
$$\begin{array}{llllll} k = n-1, & a_{n-1}, & \Delta_{n-1}, & A_{n-1}, & S_{n-1}, & b_{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ k = 1, & a_1, & \Delta_1, & A_1, & S_1, & b_1 \end{array}$$



The single-sweep algorithm

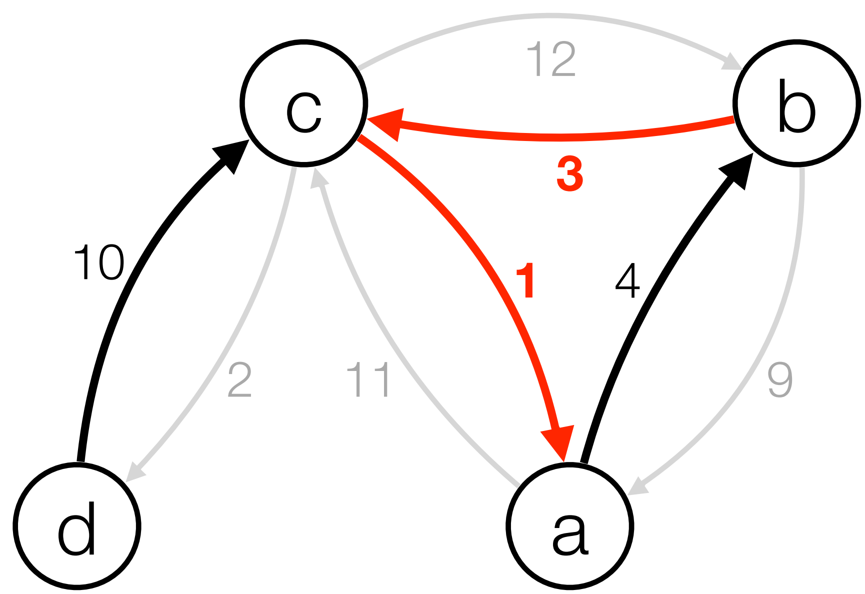
(T. Gan, C., 2015)

- Form binary trees out of sets of outgoing arcs for each vertex
- Delete the minimal outgoing arc $\mathbf{min\_arc}(i)$ from the tree of each vertex i and add it to the main tree
- While the main tree contains more than 1 arc, keep adding arcs to build optimal W-graphs

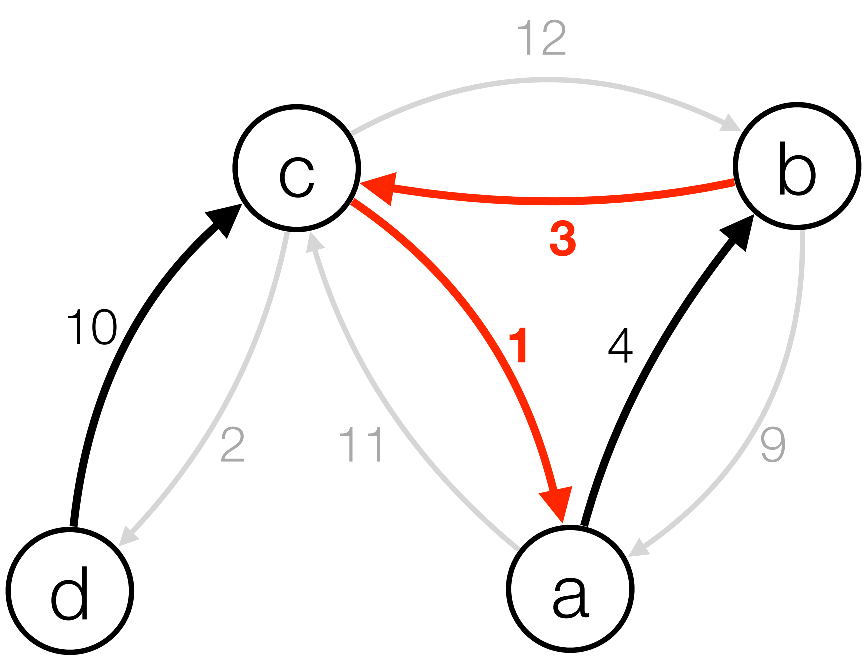


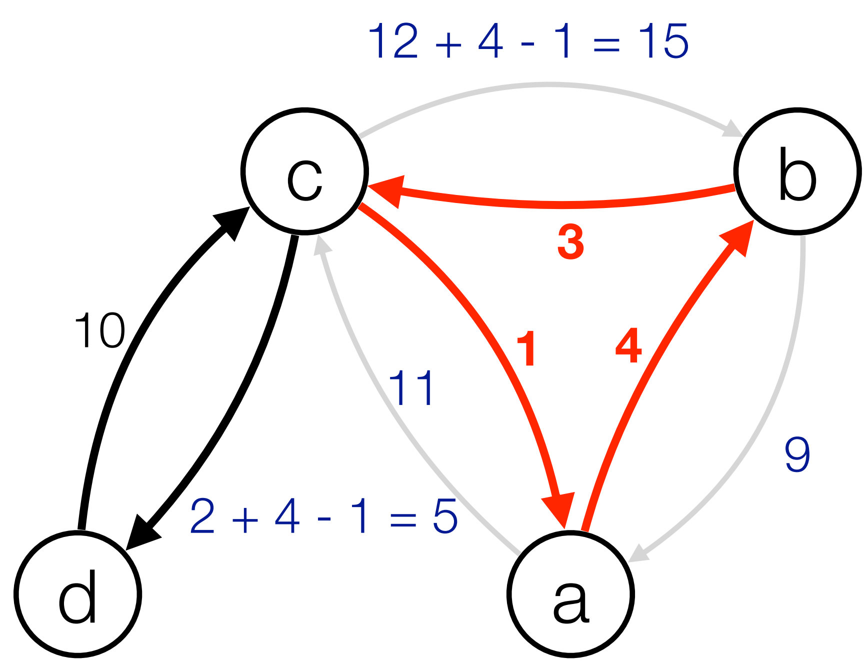
$$\Delta_3, = 1 \quad S_3 = \{c\}, \quad \mathrm{sink}_3 = c$$

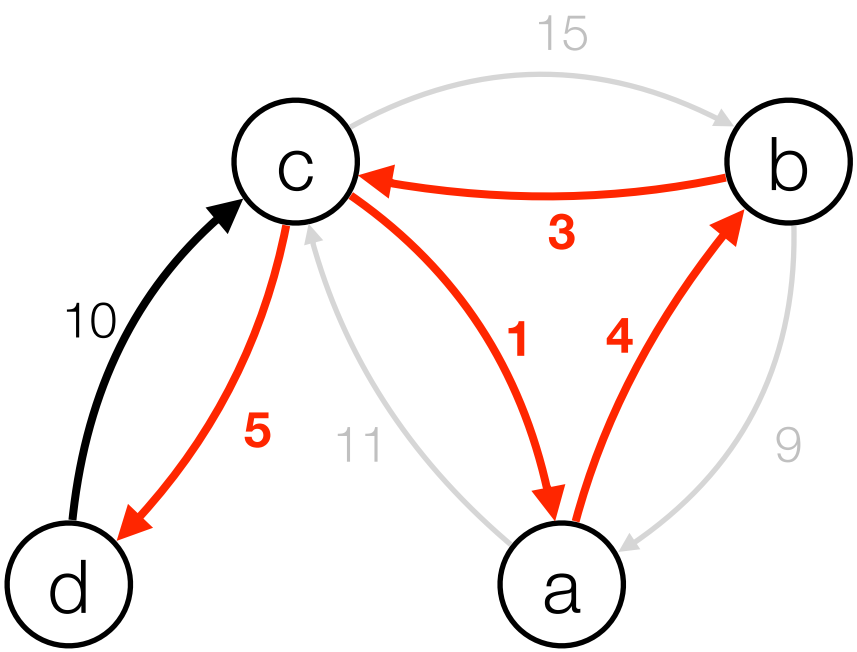
$$\Delta_2, = 3 \quad S_2 = \{b\}, \quad \mathrm{sink}_2 = b$$



- If the arc $a \to b$ on the top of the main tree creates a directed cycle, do:
  - Update *U*'s of in each tree reserve outgoing arcs of vertices lying
  - in the cycle according to the rule: $U_{ij} = U_{ij} + U_{ab} - U_{\min\_\mathrm{arc}(i)}$
  - Merge trees of remaining outgoing arcs from all vertices of the cycle
  - Keep deleting the minimal outgoing arcs $p \to q$ from the merged tree and discard it until p and q are associated with the merged tree.
  - Delete the minimal outgoing arc $p \to q$ from the merged tree and add it to the main tree.
  - For all vertices i associated with the merged tree, $\mathrm{min\_arc}(i) = p \to q$

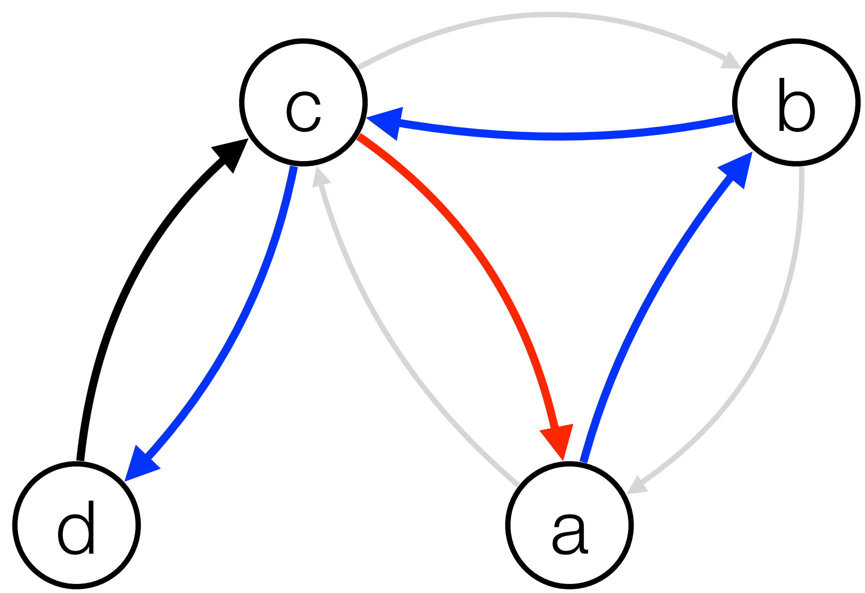






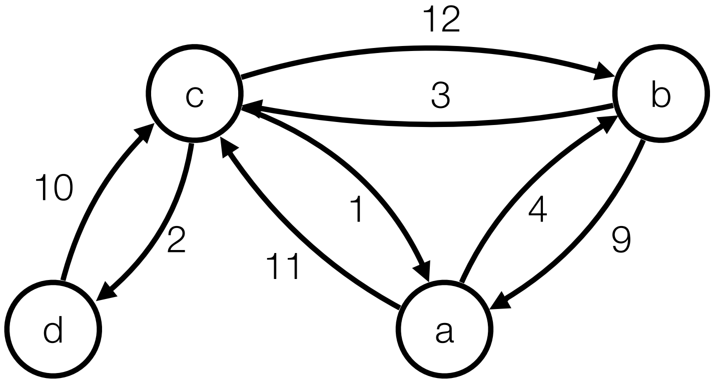
- Find optimal W-graphs:
  recursively trace arcs from
  the set that
  ever appear on the top
  of the main tree backwards
  starting from the sink, so that
  each vertex has exactly one
  outgoing arc

$$\Delta_3, = 1 \quad S_3 = \{c\}, \quad \mathrm{sink}_3 = c$$
$$\Delta_2, = 3 \quad S_2 = \{b\}, \quad \mathrm{sink}_2 = b$$
$$\Delta_1, = 5 \quad S_1 = \{a, b, c\}, \quad \mathrm{sink}_1 = a$$
$$\mathrm{sink}_0 = d$$



Blue arcs form
the optimal W-graph g_1^*

Initialization

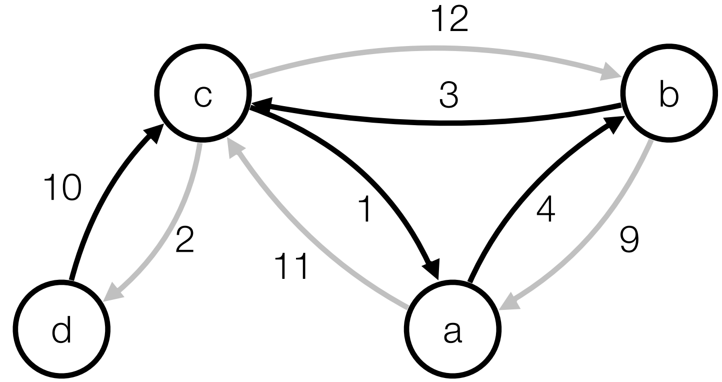


$B_a = \{[(a \to b), 4], [(a \to c), 11]\};$

$B_b = \{[(b \to c), 3], [(b \to a), 9]\};$

$B_c = \{[(c \to a), 1], [(c \to d), 2], [(c \to b), 12]\};$

$B_d = \{[(d \to c), 10]\};$

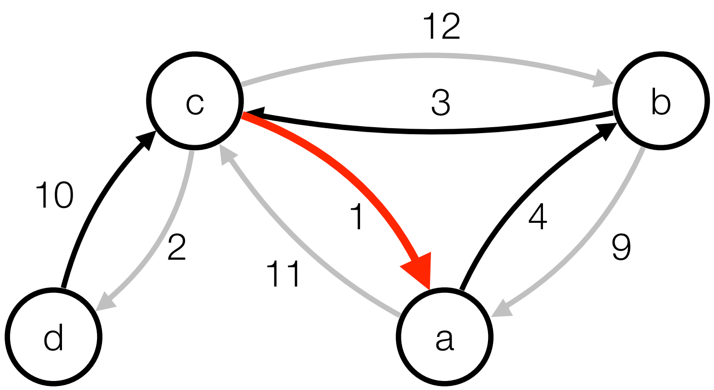


$B_a = \{[(a \to c), 11]\}; \quad B_b = \{[(b \to a), 9]\};$

$B_c = \{[(c \to d), 2], [(c \to b), 12]\}; \quad B_d = \emptyset;$

$M = \{[(c \to a), 1], [(b \to c), 3], [(a \to b), 4], [(d \to c), 10]\};$

While-cycle, step 1



$B_a = \{[(a \to c), 11]\}; \quad B_b = \{[(b \to a), 9]\};$

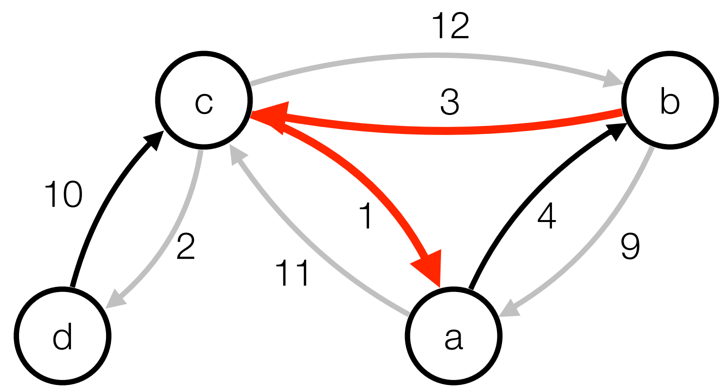
$B_c = \{[(c \to d), 2], [(c \to b), 12]\}; \quad B_d = \emptyset;$

$M = \{[(b \to c), 3], [(a \to b), 4], [(d \to c), 10]\};$

$s_3^* = c; \quad \Delta_3 = 1; \quad A_3 = a_{ca};$

$g_3^* = \{(c \to a)\};$

While-cycle, step 2



$B_a = \{[(a \to c), 11]\}; \quad B_b = \{[(b \to a), 9]\};$

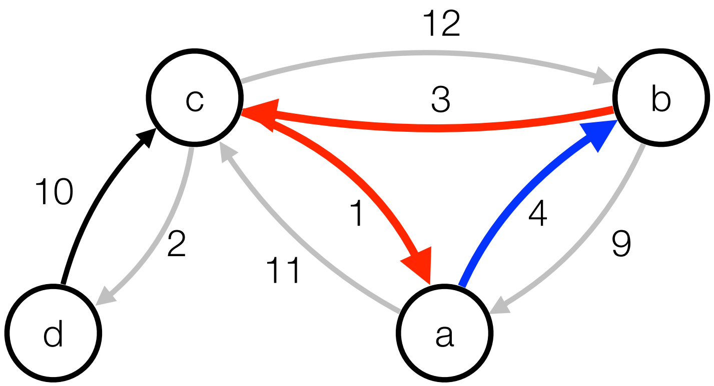
$B_c = \{[(c \to d), 2], [(c \to b), 12]\}; \quad B_d = \emptyset;$

$M = \{[(a \to b), 4], [(d \to c), 10]\};$

$s_2^* = b; \quad \Delta_2 = 3; \quad A_2 = a_{bc};$

$g_2^* = \{(c \to a), (b \to c)\};$

While-cycle, step 3



$B_a = \{[(a \to c), 11]\}; \quad B_b = \{[(b \to a), 9]\};$

$B_c = \{[(c \to d), 2], [(c \to b), 12]\}; \quad B_d = \emptyset;$

$M = \{[(d \to c), 10]\};$

Cycle $\{(a \to b), (b \to c), (c \to a)\}$ is created

Update $B_a,\ B_b,$ and B_c :

$B_a = \{[(a \to c), 11 + 4 - 4 = 11]\}; \quad B_b = \{[(b \to a), 9 + 4 - 3 = 10]\};$

$B_c = \{[(c \to d), 2 + 4 - 1 = 5], [(c \to b), 12 + 4 - 1 = 15]\};$

Merge $B_a,\ B_b,$ and B_c :

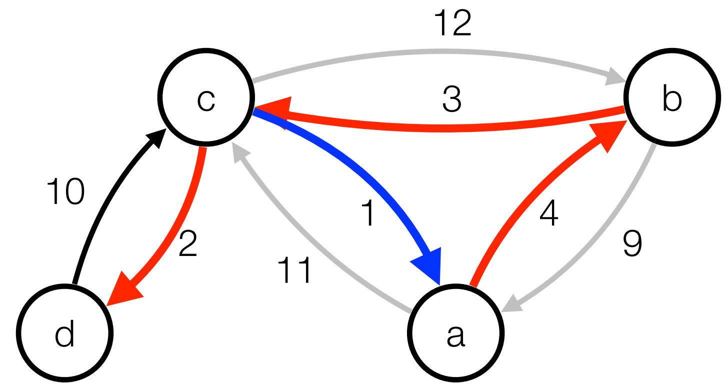
$B := \{[(c \to d), 5], [(b \to a), 10], [(a \to c), 11], [(c \to b), 15]\};$

$B_a = B_b = B_c = B;$

Remove the minimum arc from B and add it to M :

$M = \{[(c \to d), 5], [(d \to c), 10]\};$

While-cycle, step 4



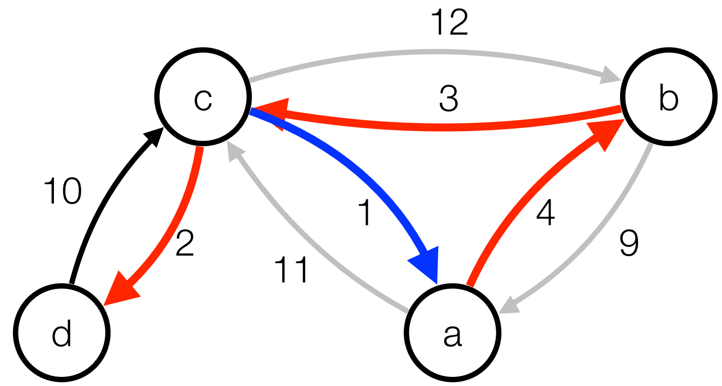
$M = \{[(d \to c), 10]\};$

$s_1^* = a; \quad \Delta_1 = 5;$

$A_1 = \dfrac{a_{cd} a_{ab}}{a_{ca}};$

$g_1^* = \{(c \to d), (b \to c), (a \to b)\}$

Results:



$$\lambda_3 \approx a_{ca} e^{-1/T}, \quad \phi_3 \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \psi_3 \approx [-1,\ 0,\ 1,\ 0]$$

$$\lambda_2 \approx a_{bc} e^{-3/T}, \quad \phi_2 \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \psi_2 \approx [-1,\ 1,\ 0,\ 0]$$

$$\lambda_1 \approx \frac{a_{cd} a_{ab}}{a_{ca}} e^{-5/T}, \quad \phi_1 \approx \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \quad \psi_1 \approx [1,\ 0,\ 0,\ -1]$$

$$\lambda_0 = 0, \quad \phi_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \psi_0 \approx [0,\ 0,\ 0,\ 1]$$

Computational cost

N vertices, index of each vertex $\leq k$

Best case scenario:

Initialization: $O(Nk \log k)$

Routine: $O(N \log N)$

Worst case scenario:

Routine: $O((Nk)^2 \log(Nk))$ due to merging trees of reserve arcs when a cycle is created

Performance

- **Lennard-Jones-38 network:** **71887** vertices, **239706** arcs
  - CPU time: **30** seconds,
  - the number of cycles encountered: **50266**
  - the number of arcs having appeared on the top of the main tree: **122152**
- **Lennard-Jones-75 network:** **169523** vertices, **441016** arcs
  - CPU time: **632** seconds (10.5 minutes)
  - the number of cycles encountered: **153164**
  - the number of arcs having appeared on the top of the main tree: **322686**

Application to Lennard-Jones-75 network

Data: courtesy of David Wales

Stats

593320 vertices, **452315** edges

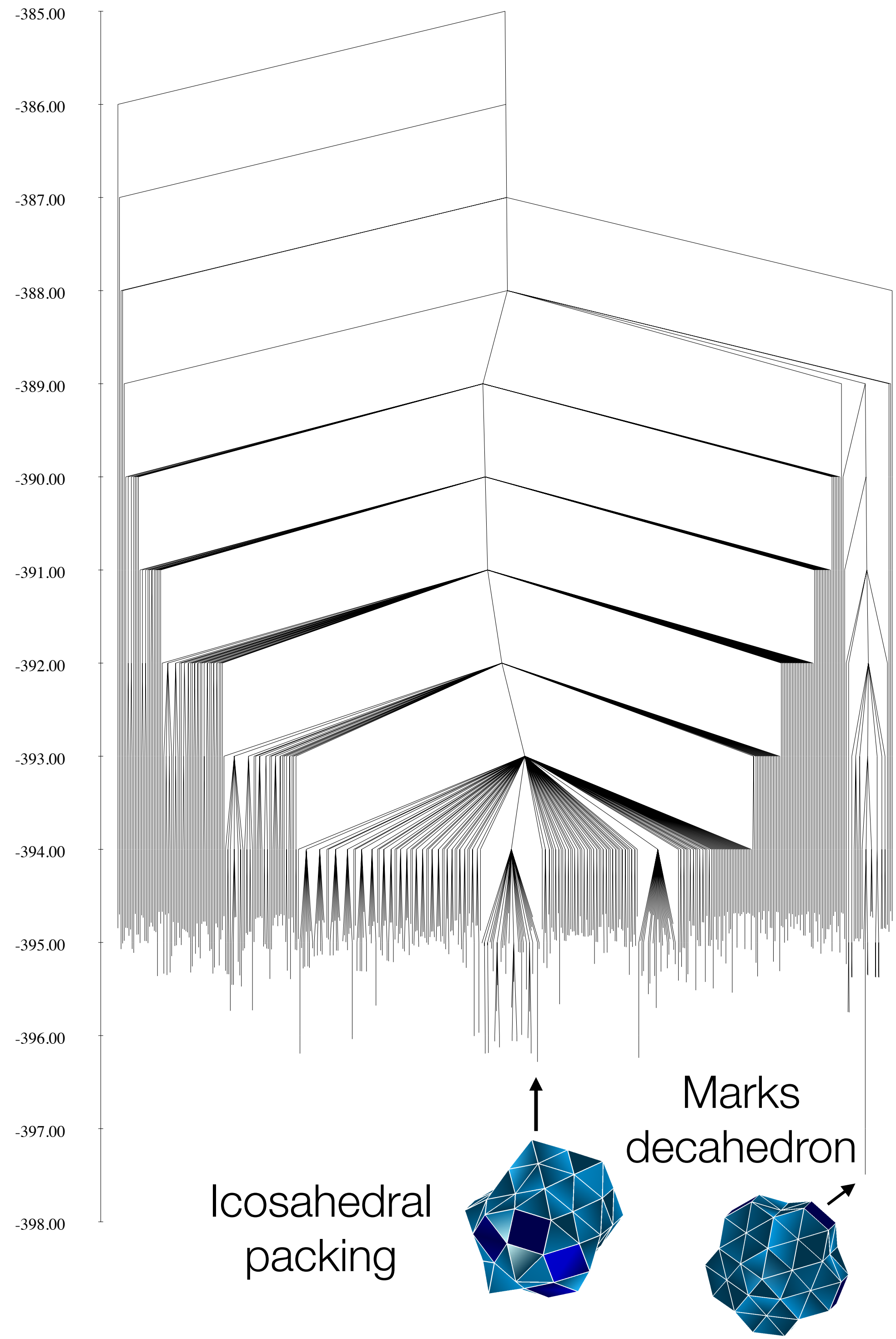
the maximal vertex index: **740**

The maximal connected component:

169523 vertices, **227198** edges

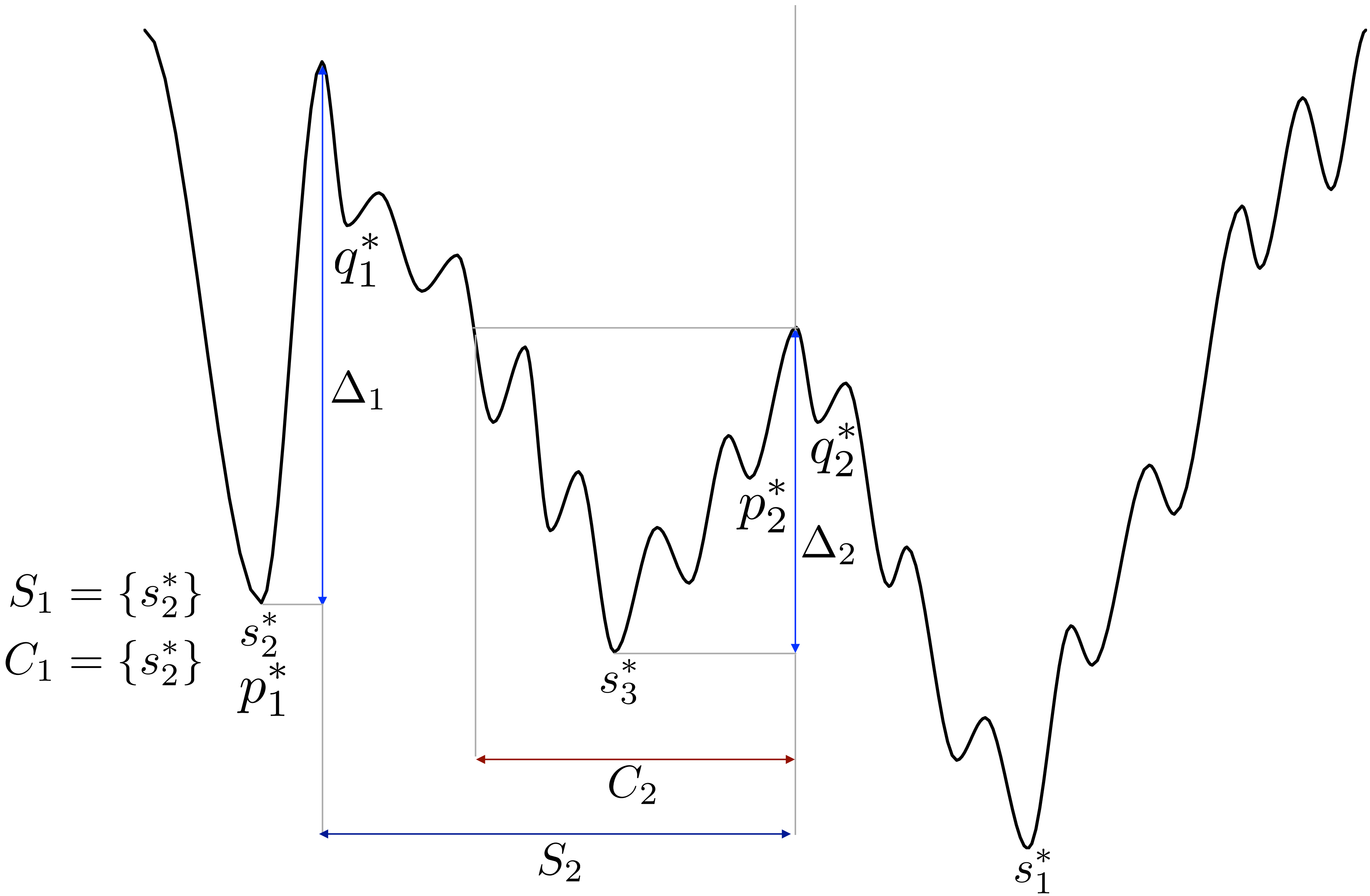
the maximal vertex degree: **740**

the number of edges that are not loops and connecting different pairs of vertices: **220508**



Zero-temperature asymptotic analysis to LJ_{75}

Quasi-invariant sets, Freidlin's cycles, etc.



Asymptotics for eigenvalues: $\lambda_k = \frac{O_{s^*_{k+1}} \bar{\nu}^{219}_{s^*_{k+1}}}{O_{p^*_k q^*_k} \bar{\nu}^{218}_{p^*_k q^*_k}} e^{-\Delta_k/T}$

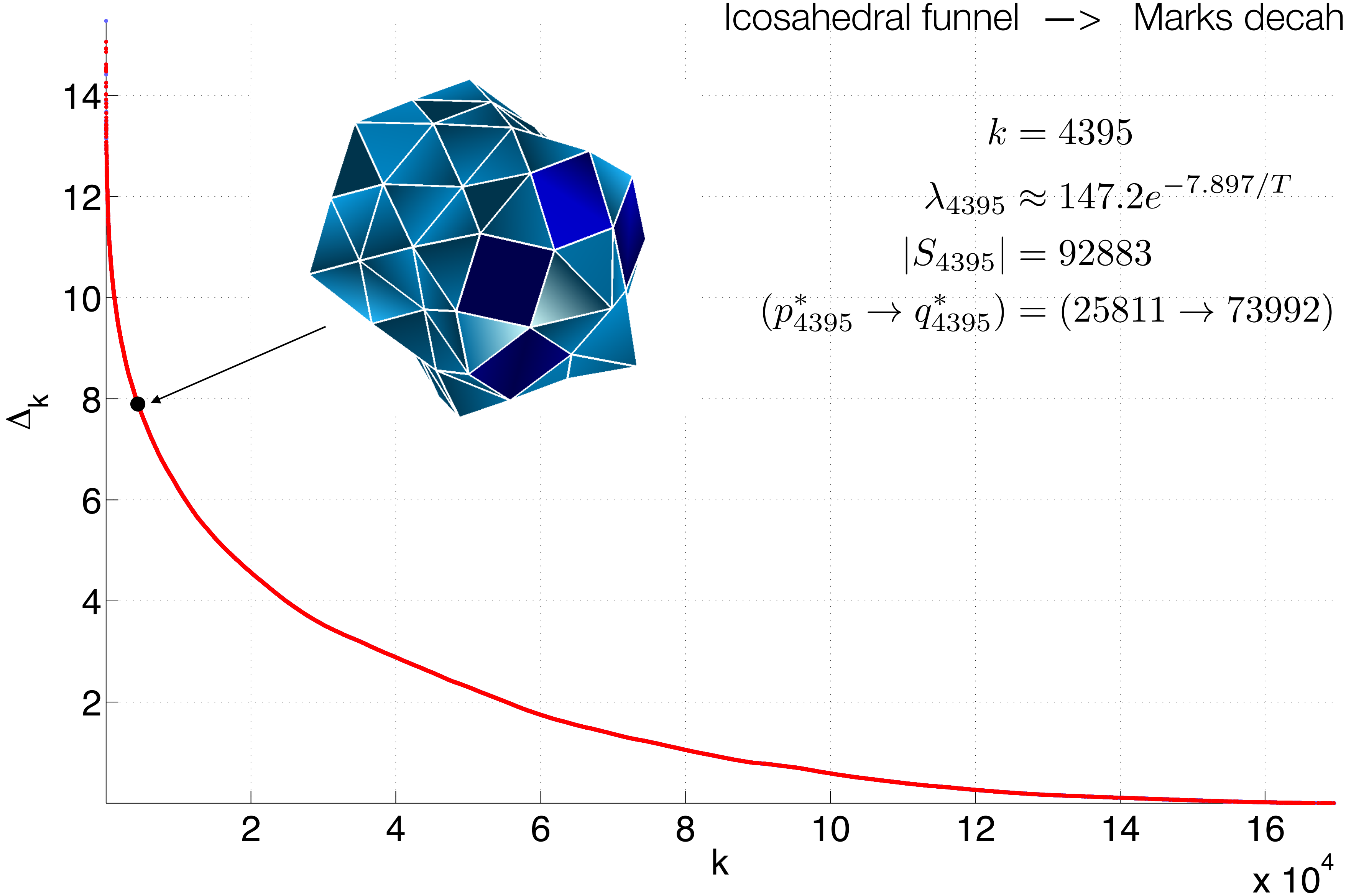
Icosahedral funnel —> Marks decahedron

$$k = 4395$$

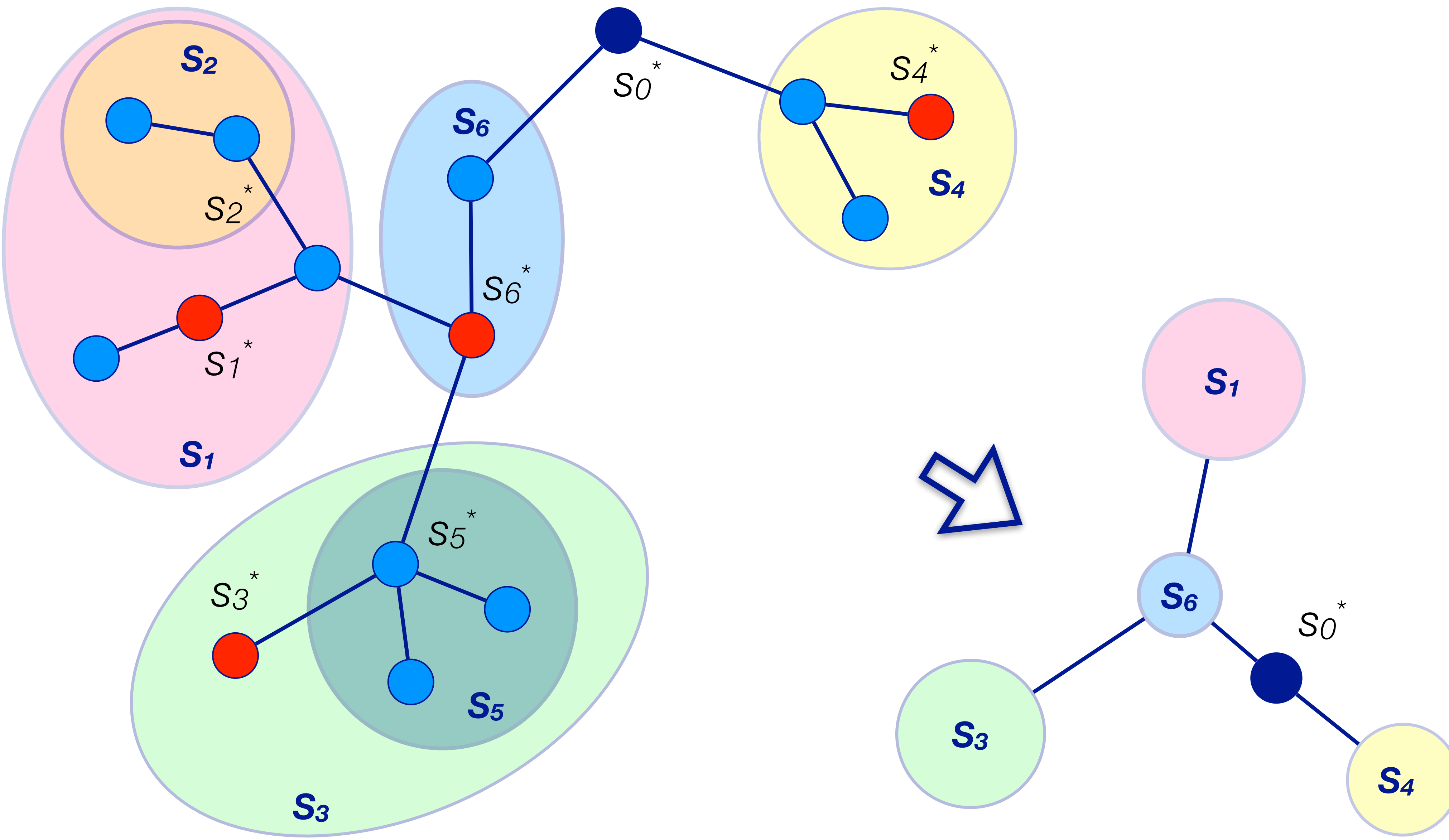
$$\lambda_{4395} \approx 147.2e^{-7.897/T}$$

$$|S_{4395}| = 92883$$

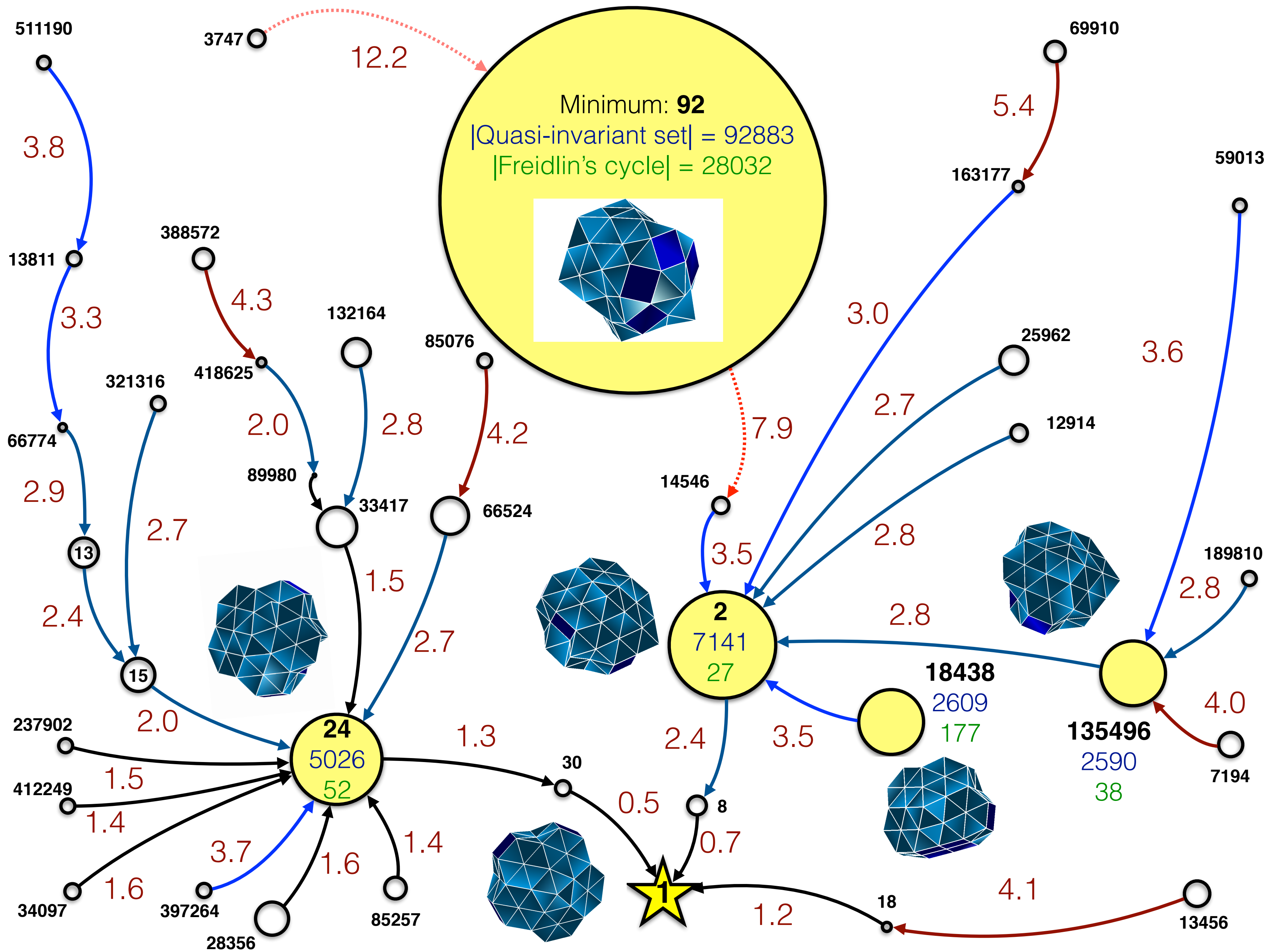
$$(p^*_{4395} \to q^*_{4395}) = (25811 \to 73992)$$



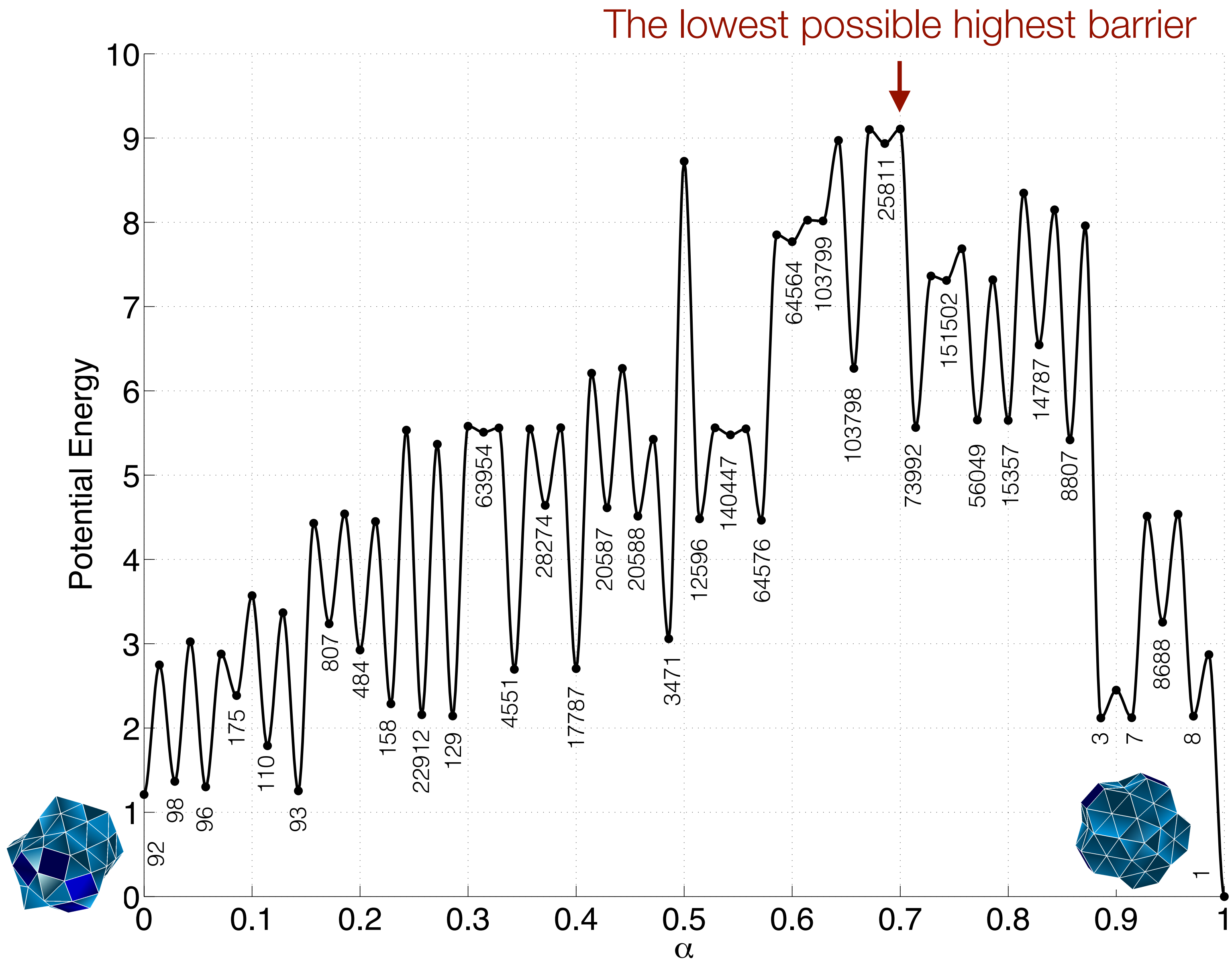
Decomposition into maximal disjoint sets S_k



Largest quasi-invariant sets (> 100 local minima)



The asymptotic zero-temperature (MinMax) path



Crystalline Order Numbers (Steinhardt, Nelson, Ronchetti, 1983)

$$Q_l = \left[\frac{4\pi}{2l+1} \sum_{m=-l}^{l} |\bar{Q}_{lm}|^2 \right]^{1/2}$$

Bond-orientational order numbers or crystalline order numbers

$$Q_{lm}(\mathbf{r}) \equiv Y_{lm}(\theta(\mathbf{r}), \phi(\mathbf{r}))$$

$Y_{lm}(\theta, \phi)$ Spherical harmonics

$\theta(\mathbf{r}),\ \phi(\mathbf{r})$ Polar angles of the bond $\mathbf{r}$

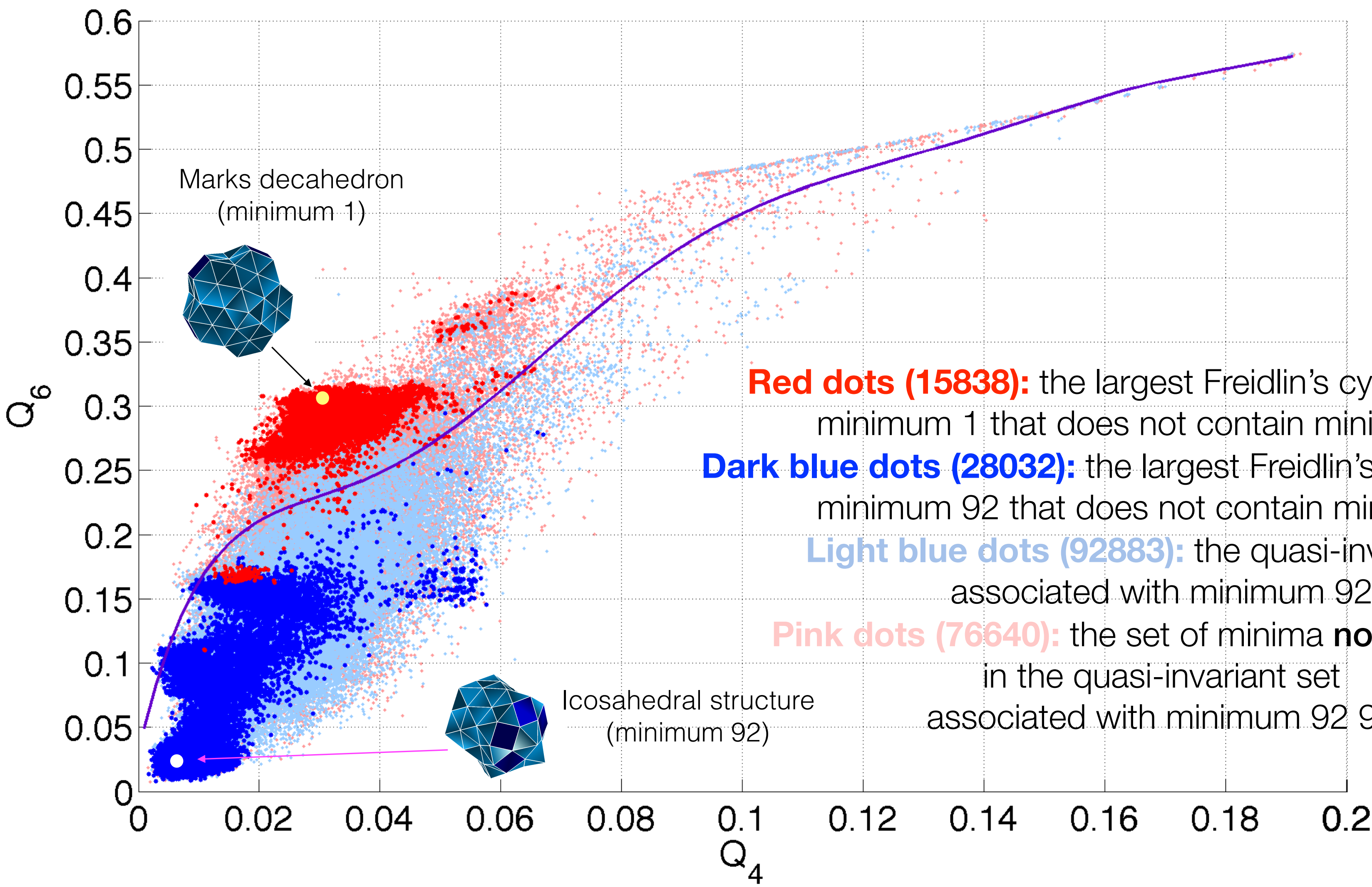
$\bar{Q}_{lm}$ Averages over all bonds in the cluster where

$$|\mathbf{r}| \leq 1.391 r^*, \quad r^* = 2^{1/6}\epsilon$$

Following Picciani, Athenes, Kurchan, Tailleur, 2011, we use

$$Q_4 \ \text{ and } \ Q_6$$

Icosahedral and Marks decahedral basins



Red dots (15838): the largest Freidlin's cycle containing minimum 1 that does not contain minimum 92.

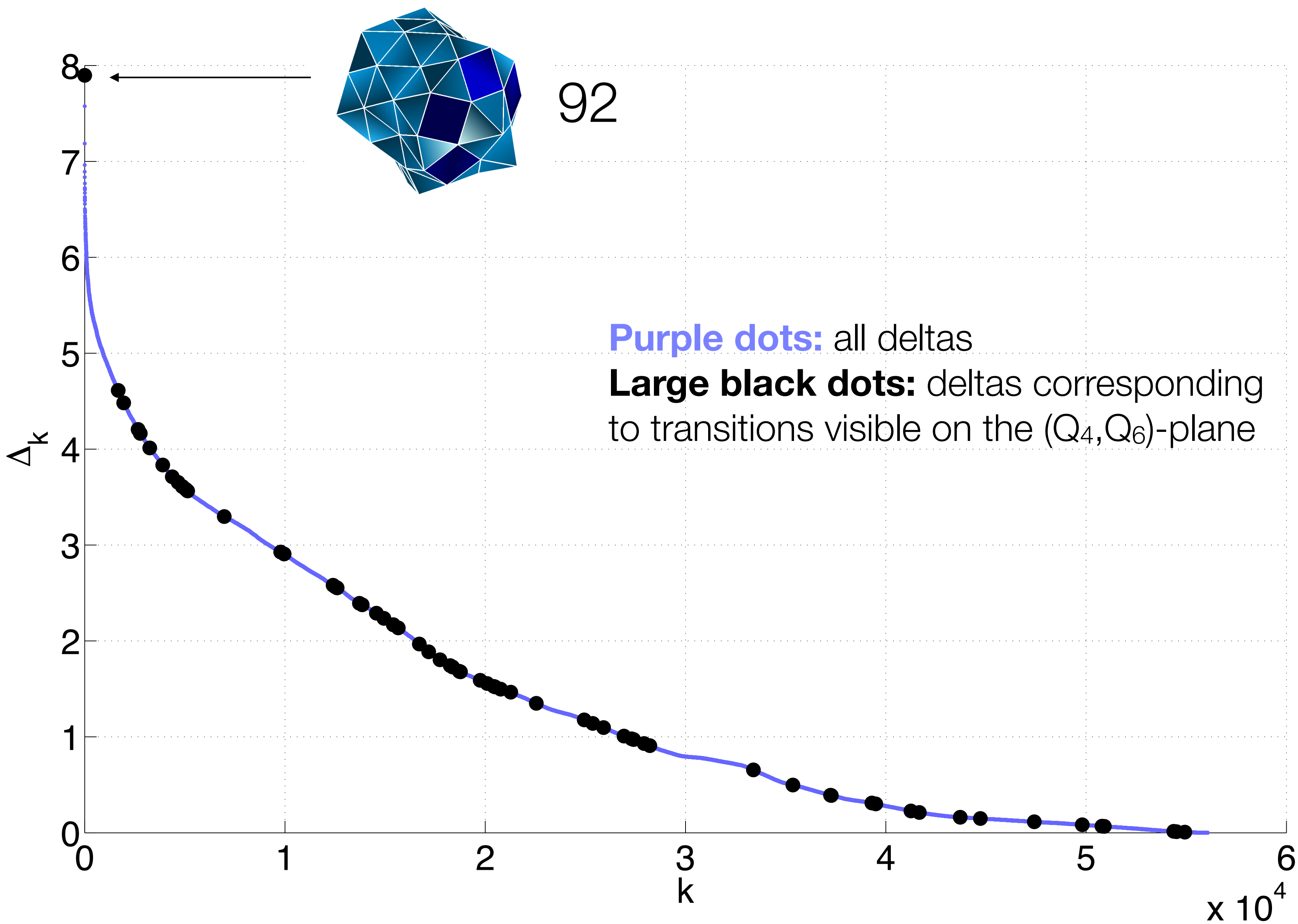
Dark blue dots (28032): the largest Freidlin's cycle containing minimum 92 that does not contain minimum 1.

Light blue dots (92883): the quasi-invariant set associated with minimum 92

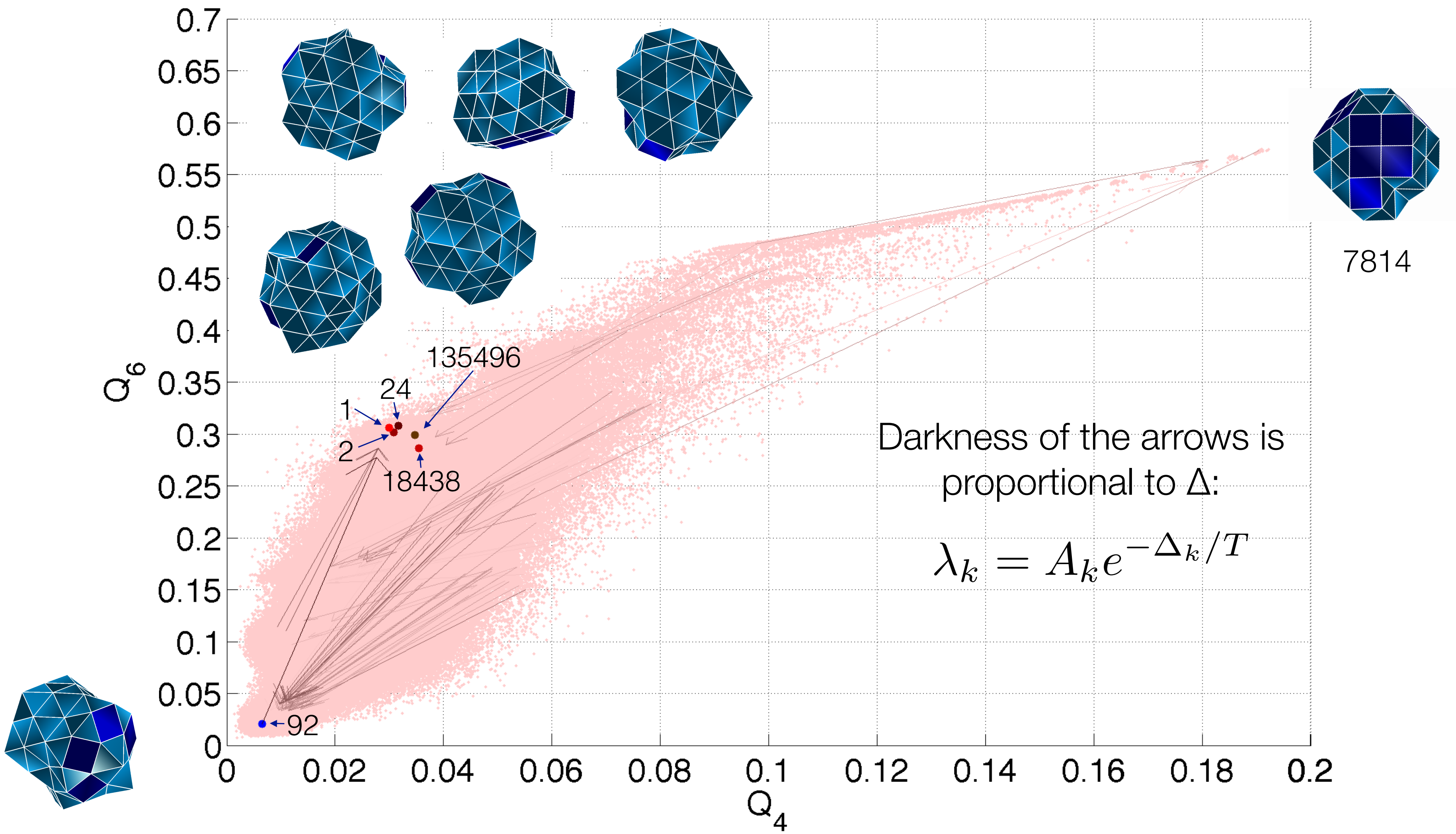
Pink dots (76640): the set of minima **not contained** in the quasi-invariant set associated with minimum 92 92

Spectrum of the truncated LJ_{75} network

($V_{max} - V_1 < \mathbf{10.0}$):   **56074** vertices, **163666** arcs



Relaxation processes visible on the (Q_4,Q_6)-plane



$$\lambda_k = A_k e^{-\Delta_k/T}$$

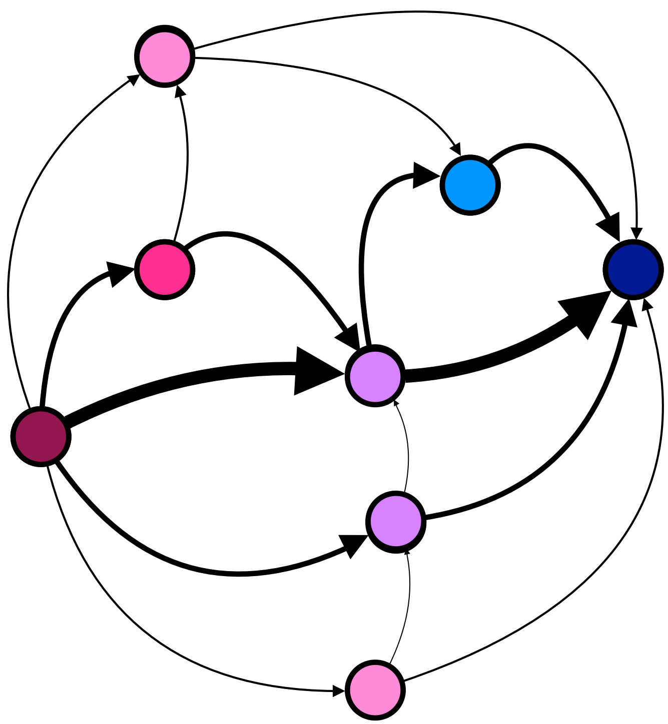
Continuation to finite temperature of λ_{4395}
which is responsible for the relaxation process
from the icosahedral funnel
to Marks decahedron funnel

Eigencurrent

$$F_{ij}^k := \pi_i L_{ij} e^{-\lambda_k t}[(\phi_k)_i - (\phi_k)_j]$$

The importance of currents was emphasized in works of J. Kurchan.

E. Vanden-Eijnden proposed to consider eigencurrents.



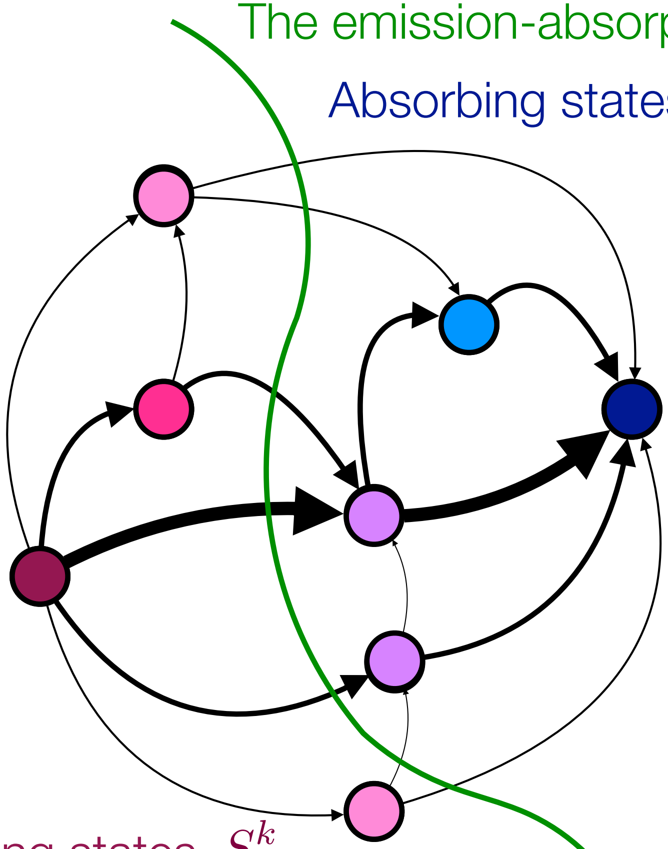
$\alpha_k F_{ij}^k$ = the net average number of transitions along the edge $(i \to j)$ per unit time at time *t* in the relaxation process from the initial distribution $\pi + \alpha_k P \phi_k$

The Fokker-Planck equation in terms of eigencurrents

$$\frac{dp_i}{dt} = -\sum_{k=0}^{n-1} c_k \sum_{j \neq i} F_{ij}^k$$

$$\sum_{j \neq i} F_{ij}^k = e^{-\lambda_k t} \lambda_k \pi_k \phi_i^k$$

The emission-absorption cut



Consider the total eigencurrent $\boldsymbol{F^k}$ through the vertex $\boldsymbol{i}$

$$\sum_{j\neq i} F_{ij}^k = \boxed{e^{-\lambda_k t}\lambda_k \pi_k} \boxed{\phi_i^k}$$

always > 0 > 0 or < 0

$$S = S_+^k \cup S_-^k$$

$$S_+^k := \{i \in S \;:\; (\phi_k)_i \geq 0\}$$

$$S_-^k := \{i \in S \;:\; (\phi_k)_i < 0\}$$

Among all possible cuts, the eigencurrent F^k is maximal through the emission-absorption cut

Ref.: M. Cameron, J. Chem. Phys. (2014), 141, 184113, arXiv: 1408.5630

Continuation of eigenpairs to finite temperatures

- ***Difficulties:*** (1) eigenvalues are close to 0 and may cross; (2) the matrix is large with widely varying entries

- ***Useful fact:*** the eigenvectors of the symmetrized generator matrix $L_{sym} := P^{1/2}LP^{-1/2} \equiv P^{-1/2}QP^{-1/2}$ are orthonormal

- ***Rayleigh Quotient iteration*** with initial approximation

$$(\psi_k^0)_i = \begin{cases} \sqrt{\pi_i}, & i \in S_k \\ 0, & i \notin S_k \end{cases}$$

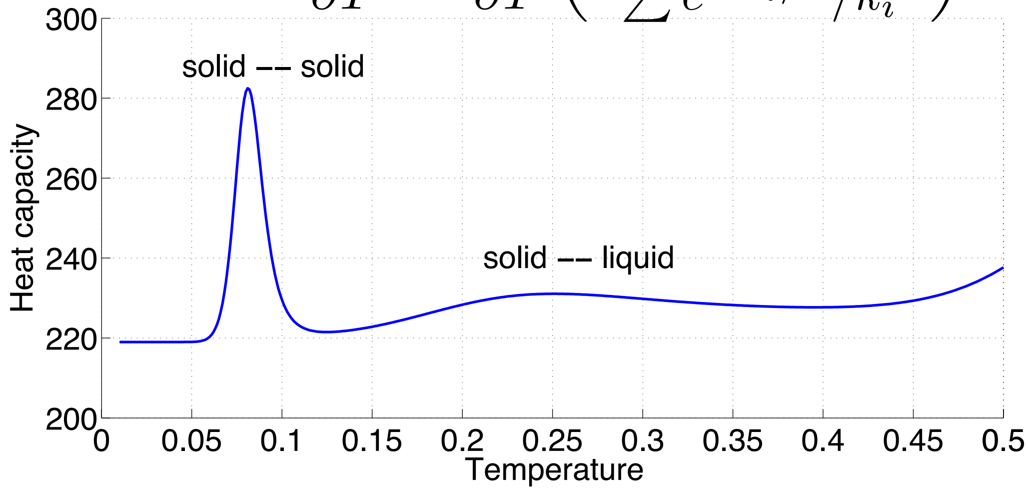
- ***Precaution:*** check whether the corresponding eigencurrent is largely emitted at the sink s_k^* and largely absorbed at the sink t_k^*

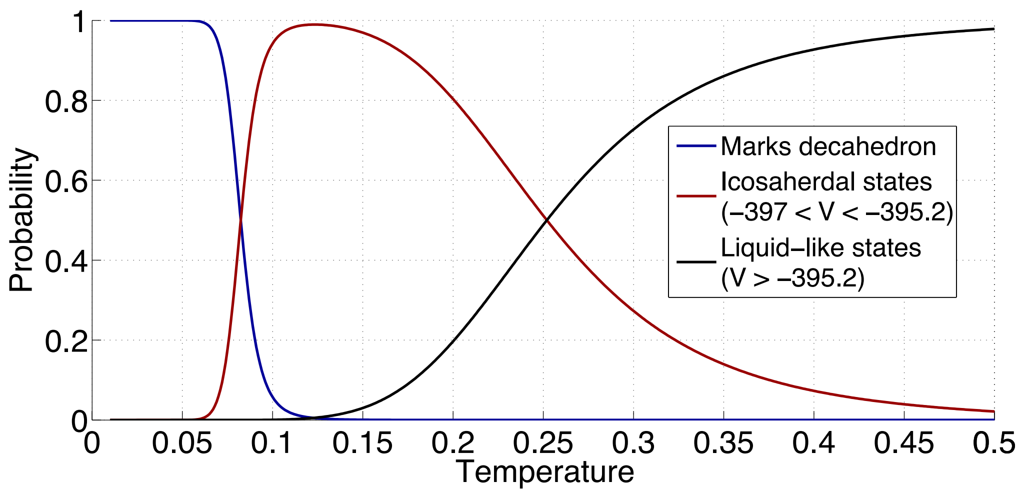
Rayleigh Quotient Iteration

```
rayleigh = @(x) x'*Lsym*x/(x'*x); % the Rayleigh quotient

rtol = 1e-6;
itermax = 12;

%% Rayleigh quotient iteration
    iter = 0;
    while abs(res) > rtol*abs(lam) & iter < itermax
        A = Lsym  - lam*speye(n);
        w = (A)\v;
        v = w/norm(w);
        res = norm(A*v);
        lam = rayleigh(v);
        iter = iter + 1;
        fprintf('iter = %d:  lam = %d\t res = %d\n',iter,lam,res);
    end
```

Difficulties with Lennard-Jones-75

$$c_v = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T}\left(\frac{\sum E_i e^{-E_i/T}/k_i}{\sum e^{-E_i/T}/k_i}\right)$$





Marks decahedron - icosahedral states
solid - solid transition: $T = 0.08$

Icosahedral - liquid-like states
transition: $T = 0.25$

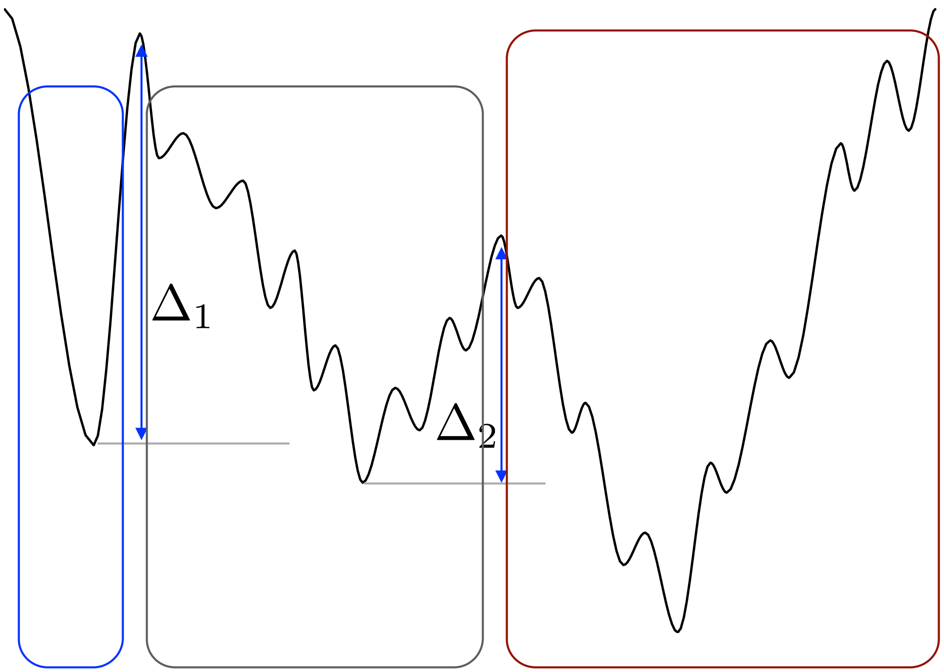
The range of temperatures to which
we would like to continue λ_{4395} :

$$0.05 \leq T \leq 0.25$$

For $T < 0.17$, the matrix is badly
scaled, and the results are
inaccurate or NaN

For $T \geq 0.17$, convergence
to a wrong eigenpair takes place

Remedy 1: lumping



Pick $\Delta_{\min}$. Here $\Delta_{\min} = \Delta_2$

Lump the quasi-invariant sets with $\Delta_k < \Delta_{\min}$

Re-calculate pairwise rates S_k

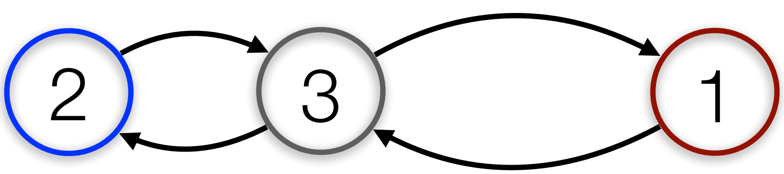
$$\tilde{L}_{kl} = \sum_{i \in S_k, j \in S_l} L_{ij} \frac{\pi_i}{\sum_{i' \in S_k} \pi_{i'}}$$

The resulting generator matrix $\tilde{L}$ is smaller, the largest entries of L are gone

$$\tilde{L}_{N \times N} = A_{N \times n} \; L_{n \times n} \; B_{n \times N}$$

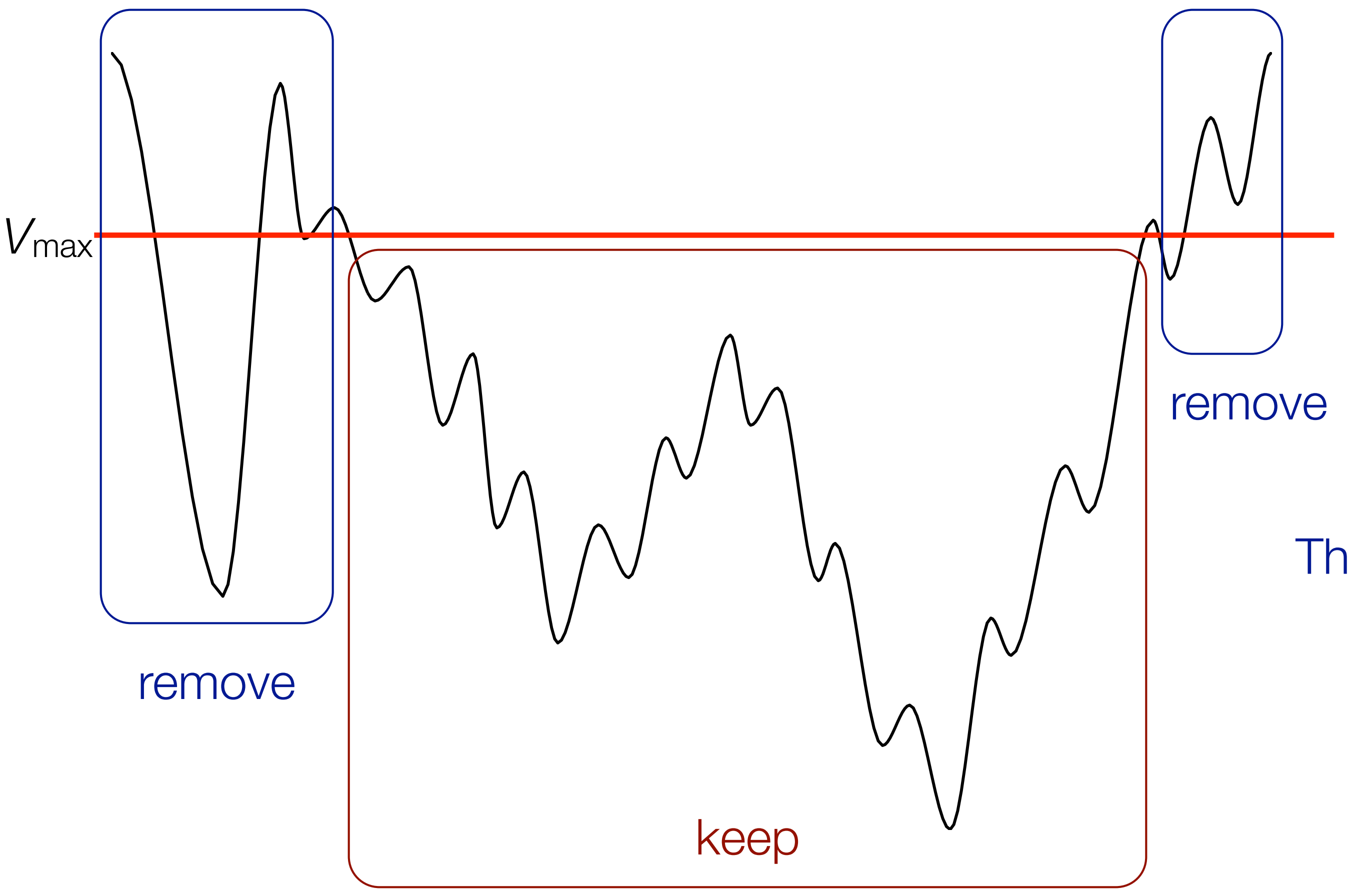
$$A_{ki} = \begin{cases} \frac{\pi_i}{\sum_{i' \in S_k} \pi_{i'}}, & i \in S_k \\ 0, & \text{otherwise} \end{cases}$$

$$B_{jl} = \begin{cases} 1, & j \in S_l \\ 0, & \text{otherwise} \end{cases}$$



The lumped network

Remedy 2: truncation

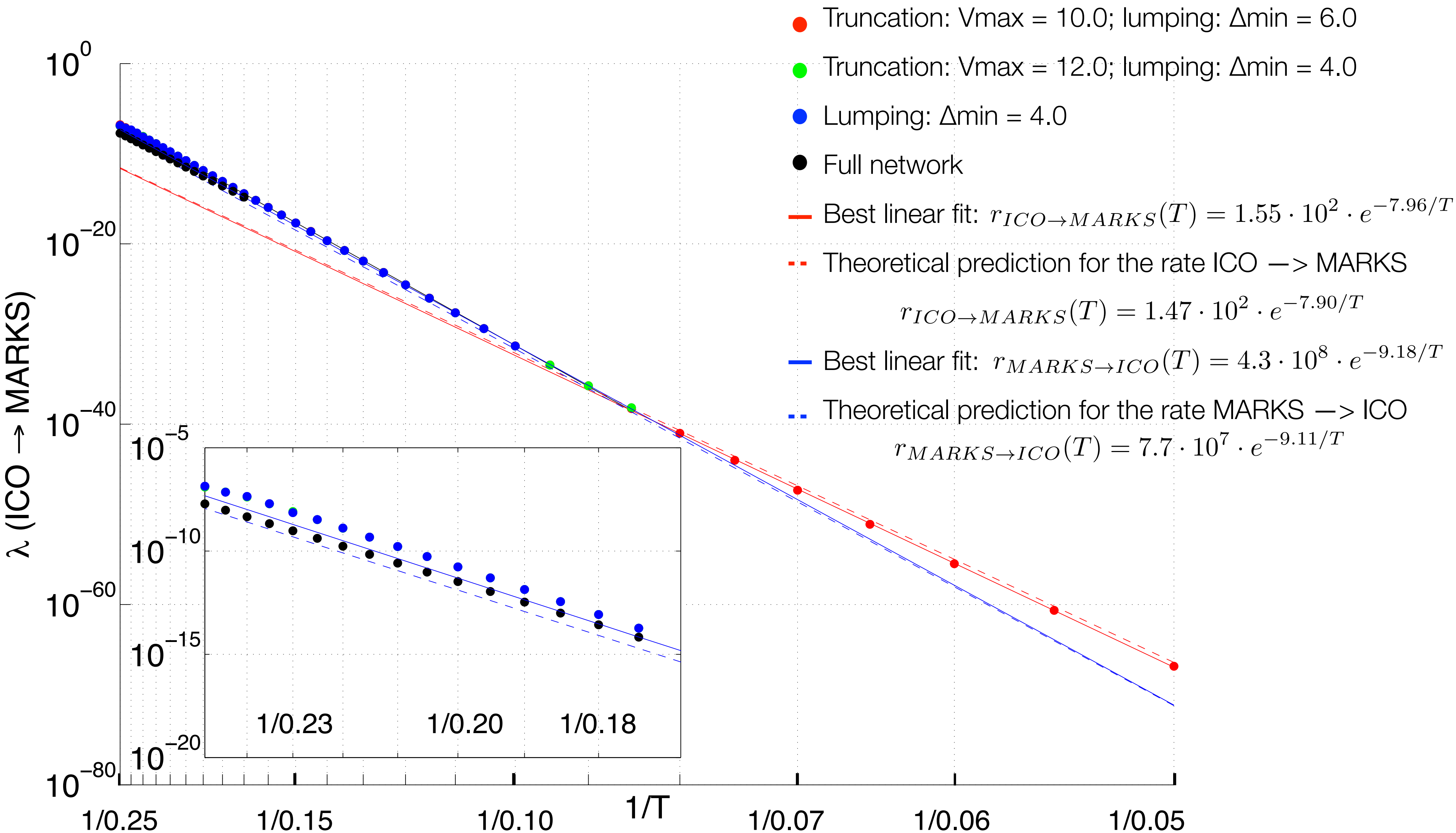


Pick V_{max}, remove all states separated from the global minimum by a barrier exceeding V_{max}

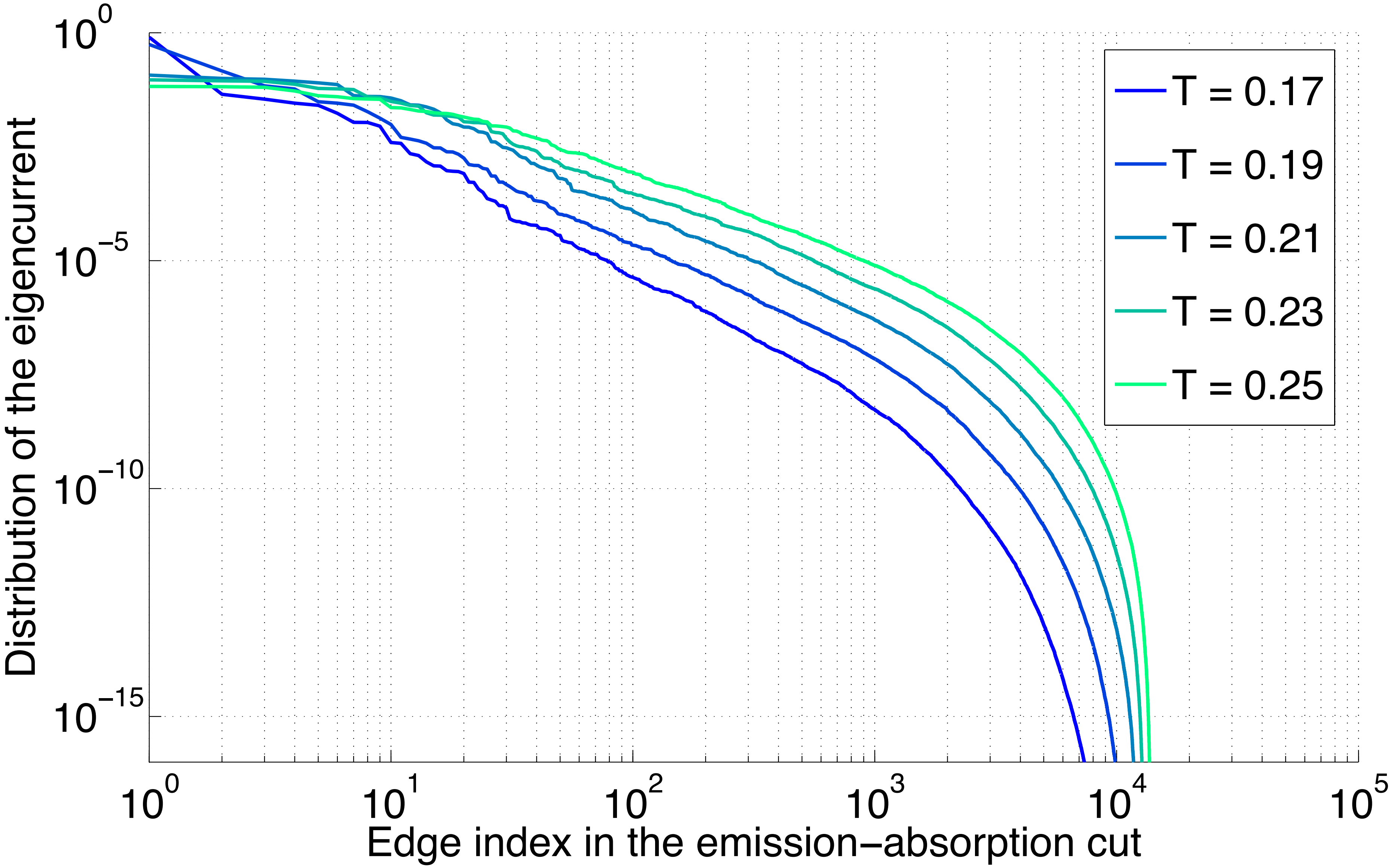
The resulting network is smaller, the components that used to be nearly transient or make it nearly reducible are removed

One can combine truncation and lumping: first truncate, then lump.

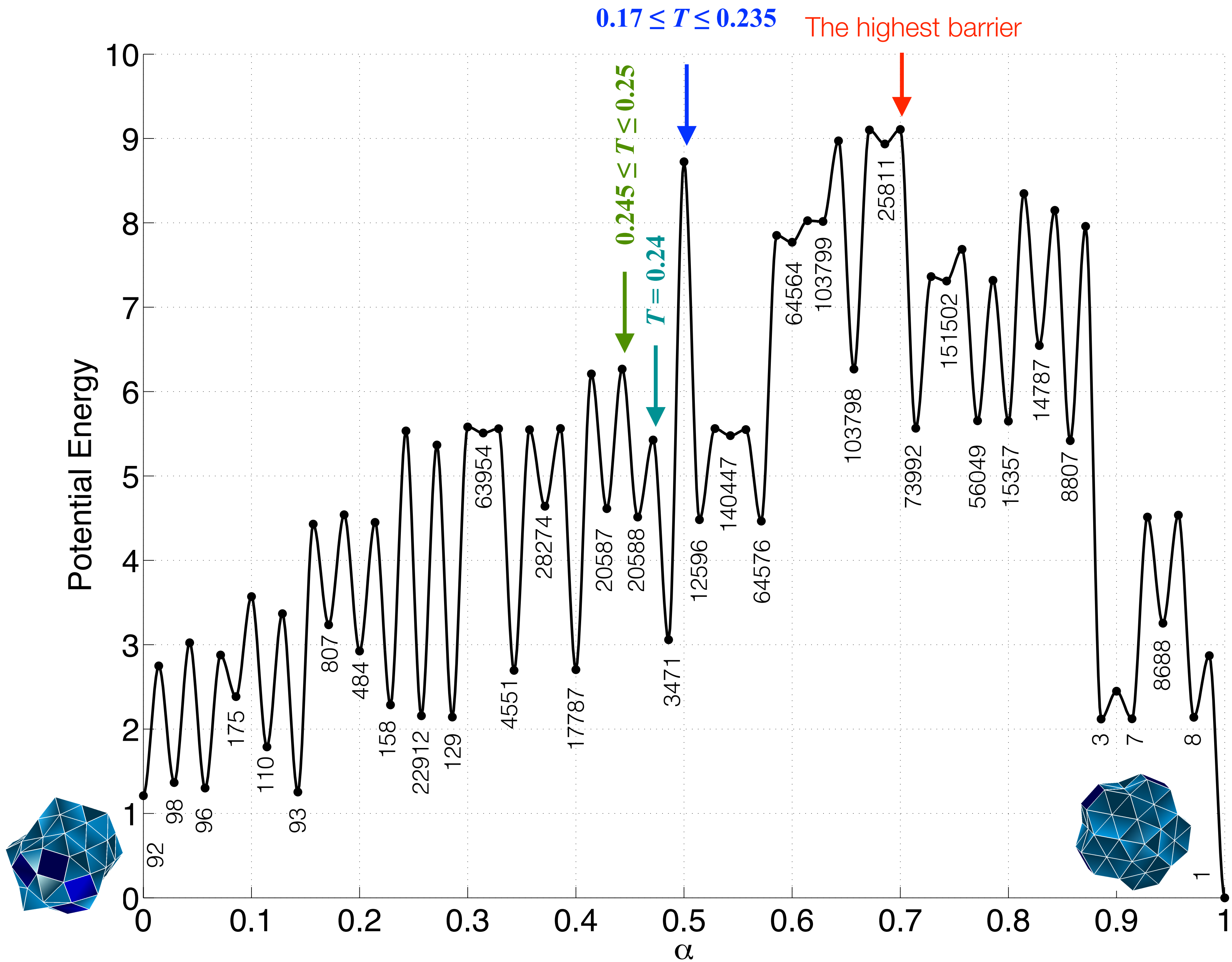
Eigenvalue λ_{4395} of LJ_{75}



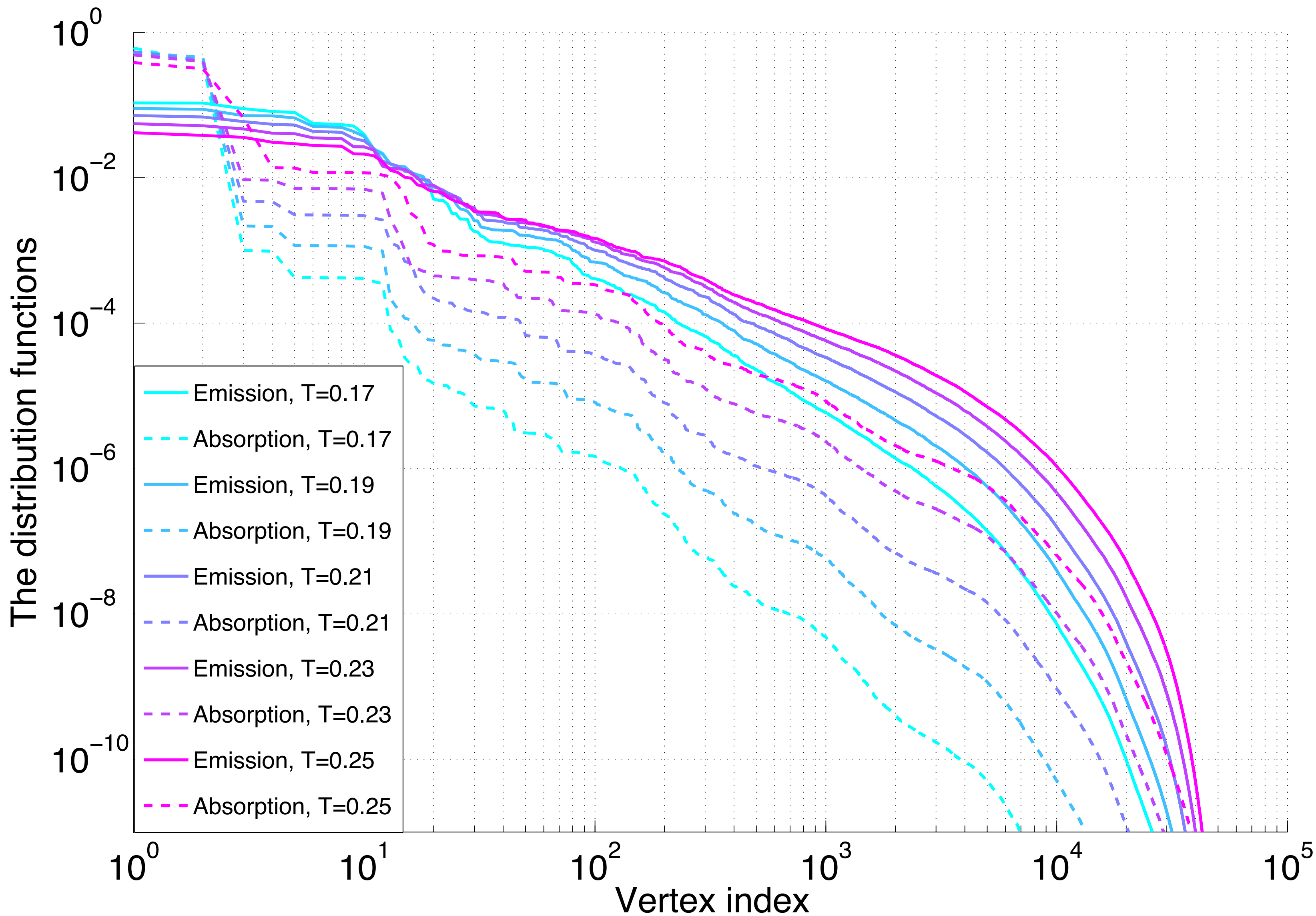
Eigencurrent distribution in the emission-absorption cut



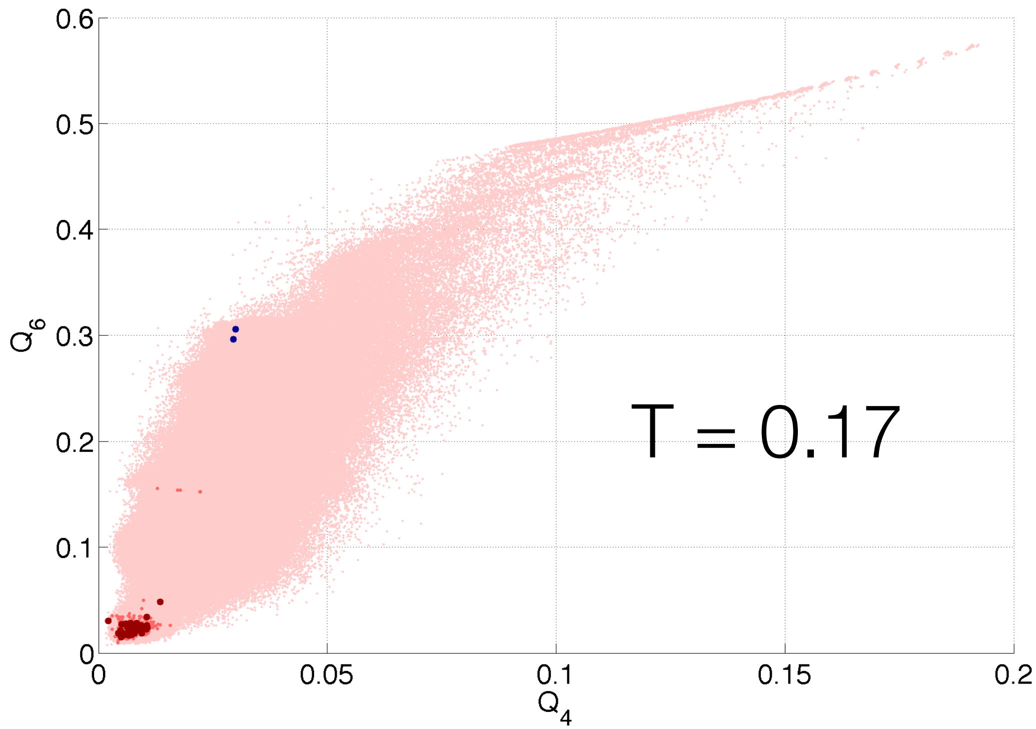
The emission-absorption cut: location

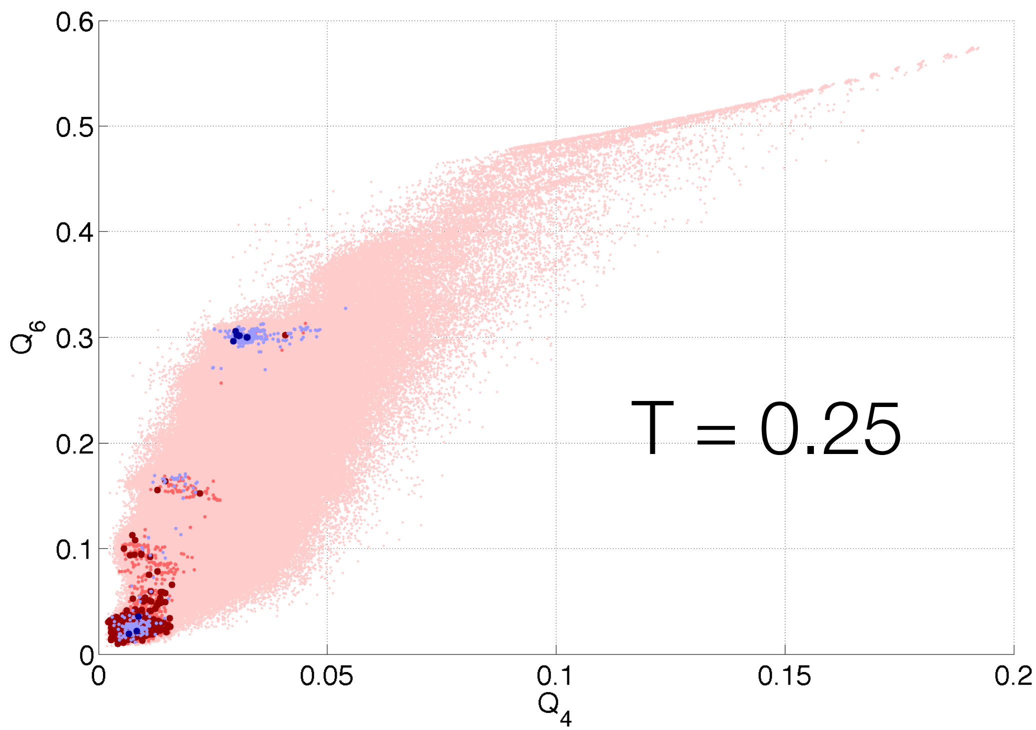


Emission-absorption distribution



Emission - absorption





- States emitting 99% of the eigencurrent
- States emitting 90% of the eigencurrent
- States absorbing 99% of the eigencurrent
- States absorbing 90% of the eigencurrent

Highlights

- Formulas for asymptotic eigenvalues: exponents and prefactors
- Nested property of optimal W-graphs for stochastic networks with pairwise transition rates of the form $L_{ij} = k_{ij} \exp(-U_{ij}/T)$
- A single-sweep algorithm for computing asymptotic eigenvalues and eigenvectors
- Application to Lennard-Jones-75

Acknowledgements

- David Wales (Cambridge University, UK)